

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS EXPRESS		FEBRUARY 08	CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:00:57 ON 11 JUN 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:01:10 ON 11 JUN 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2

DICTIONARY FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

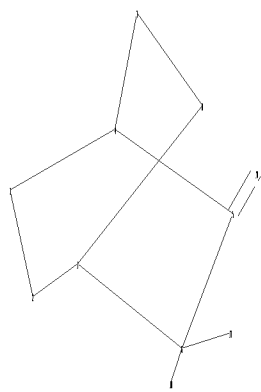
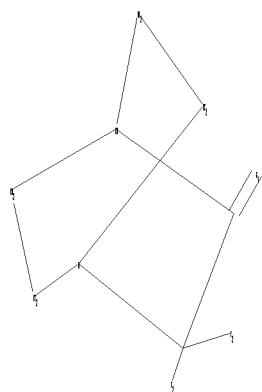
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10590054.str



```

chain nodes :
10 12 13 17 18
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
5-10 6-17 6-18 12-13
ring bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 7-8
exact/norm bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 5-10 6-17 6-18 7-8 12-13

```

G1:O,S,N

G2:H, [*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 12:CLASS
13:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

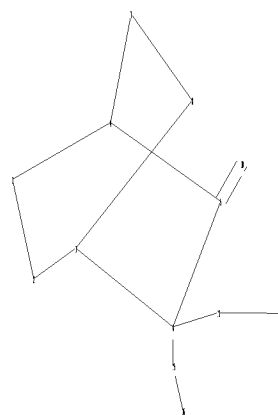
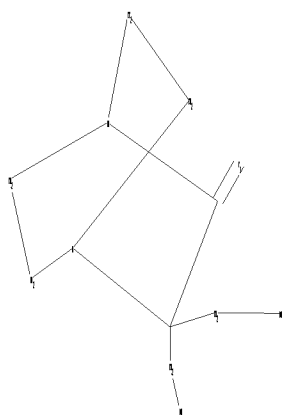
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10590054b.str



```

chain nodes :
10 13 14 15 16
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
5-10 6-13 6-15 13-14 15-16
ring bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 7-8
exact/norm bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 5-10 7-8
exact bonds :
6-13 6-15 13-14 15-16

```

G1:O,S,N

G2:H

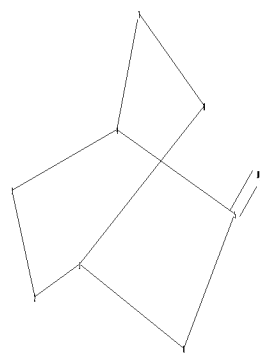
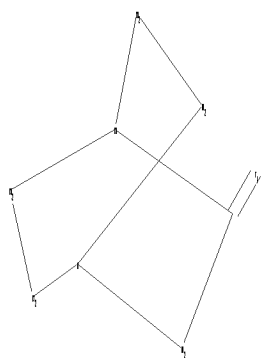
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 13:CLASS
14:CLASS 15:CLASS 16:CLASS

L2 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10590054c.str



```

chain nodes :
10
ring nodes :
1  2  3  4  5  6  7  8
chain bonds :
5-10
ring bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  7-8
exact/norm bonds :
5-10
exact bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  7-8

```

isolated ring systems :
containing 1 :

G1:O,S,N

G2:H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS

L3 STRUCTURE UPLOADED

=> s l1 full

FULL SEARCH INITIATED 15:02:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 84668 TO ITERATE

100.0% PROCESSED 84668 ITERATIONS

925 ANSWERS

SEARCH TIME: 00.00.01

L4 925 SEA SSS FUL L1

=> s l2 full

FULL SEARCH INITIATED 15:03:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L5 2 SEA SSS FUL L2

=> s l3 full

FULL SEARCH INITIATED 15:03:08 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 46039 TO ITERATE

100.0% PROCESSED 46039 ITERATIONS

436 ANSWERS

SEARCH TIME: 00.00.01

L6 436 SEA SSS FUL L3

=> s l4 not l5 full

L7 923 L4 NOT L5

=> s l7 not l6 full

L8 487 L7 NOT L6

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

536.00

536.21

FILE 'CAPLUS' ENTERED AT 15:04:27 ON 11 JUN 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 11 Jun 2008 VOL 148 ISS 24
FILE LAST UPDATED: 10 Jun 2008 (20080610/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s l8 full
L9 160 L8

=> d ibib abs hitstr 160

L9 ANSWER 160 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1940:708 CAPLUS

DOCUMENT NUMBER: 34:708

ORIGINAL REFERENCE NO.: 34:110b-g

TITLE: Synthesis of 5-substituted rubans

AUTHOR(S): Clemo, G. R.; Hoggarth, E.

SOURCE: Journal of the Chemical Society (1939) 1241-4

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 34:708

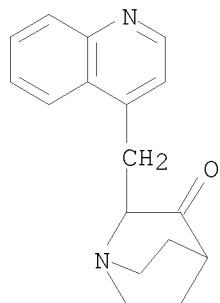
GI For diagram(s), see printed CA Issue.

AB Lepidine (40 g.), 44 g. chloral and 100 cc. C₅H₅N, warmed at 85-90° for 2 hrs., give 80% of γ -trichloro- β -hydroxy- α -(4-quinolyl)propane, m. 178°; adding 65 g. during 2 hrs. to 65 g. KOH in 300 cc. absolute EtOH on the water bath gives 80% of β -4-quinolylacrylic acid, m. 270°; oxidation of 36 g. acid in a solution of 14 g. Na₂CO₃ in 500 cc. H₂O with 60 g. KMnO₄ in 1.5 l. H₂O at -10° gives 58% (overall yield 38-40%) of quinoline-4-aldehyde (I), b₄ 122-3°, m. 52°; picrate, yellow, m. 179° (contains 1 mole of EtOH). 3-Ketoquinuclidine (II) (C. and Metcalfe, C. A. 32, 1701.3, term it the 2-derivative) and BzH in absolute EtOH containing piperidine or KOH, refluxed 8-10 hrs., give 2-benzylidene-3-ketoquinuclidine, light yellow, m. 133°; phenylhydrazone, light yellow, m. 184°. II (0.5 g.) and 0.8 g. I in AcOH, saturated with dry HCl at 0°, and after 2-3 hrs. warmed at 80-5° for 8 hrs., give 0.2 g. 5-keto-6,9-rubanene (III), deep yellow, m. 153°; III results in 0.4-0.5 g. yield from 0.5 g. II and 0.65 g. I with piperidine acetate in absolute EtOH; after keeping 60 hrs. in the cold and then heating momentarily to boiling; picrate, red, m. 209°; chloroplatinate, orange needles, decompose above 260° without melting. Catalytic reduction of 0.5 g. of III with Pd-C in MeOH gives 0.3 g. of 5-ketoruban (IV (R = 4-quinolyl)), m. 125-6°; phenylhydrazone, yellow, m. 198°; picrate, deep yellow, m. 168°. Reduction of 0.5 g. of IV with (iso-PrO)₃Al in iso-PrOH gives 0.3 g. of ruban-5-ol, m. 198°; picrate, yellow, m. 188-9°. IV (0.3 g.) with EtMgI in Et₂O at -10° gives 0.03-0.05 g. of 5-ethylruban-5-ol (V), m. 139°; picrate, yellow, m. 161°. III (0.8 g.) and EtMgI in Et₂O at 0° give 0.05 g. of a compound C₁₉H₂₂ON₂, m. 164°; picrate, deep yellow, m. 150°; crystalline compds. could not be prepared with N₂H₄.H₂O, PhNHNH₂, NH₂OH or H₂NNHCONH₂; no Me₂CO was detected in an attempted reduction with (iso-PrO)₃Al and the compound was unchanged on boiling with HCO₂H or Ac₂O; catalytic reduction did not yield V.

IT 24177-70-6, 3-Quinuclidinone, 2-(4-quinolylmethyl)-
(and derivs.)

RN 24177-70-6 CAPLUS

CN 11-Norcinchonan-7-one, (8 ξ)-(9CI) (CA INDEX NAME)



=> d ibib abs hitstr 150-159

L9 ANSWER 150 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:430341 CAPLUS

DOCUMENT NUMBER: 71:30341

ORIGINAL REFERENCE NO.: 71:5589a,5592a

TITLE: Antimalarials. Some quinuclidine derivatives of 7-chloro-4-aminoquinoline and 6-methoxy-8-aminoquinoline

AUTHOR(S): Singh, Tara; Stein, Robert G.; Koelling, Harlan H.; Hoops, John F.; Biel, John H.

CORPORATE SOURCE: Res. Lab., Aldrich Chem. Co., Inc., Milwaukee, WI, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12, 524-6

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Thirteen quinoline compds. containing quinuclidine rings in side chains were prepared and tested for their antimalarial activity against Plasmodium berghei in mice. 7-Chloro-4-(3-oxoquinuclidinyl-2-methyleneamino)quinoline (I) and 7-chloro-4-(3-hydroxyquinuclidinyl-2-methyleneamino)quinoline (II) were curative; I cured 2 mice at 160 mg./kg. and all 5 in the test at 640 mg./kg., while II showed slight activity at 160 and 320 mg./kg. and cured all 5 mice at 640 mg./kg. All other compds. were inactive and toxic.

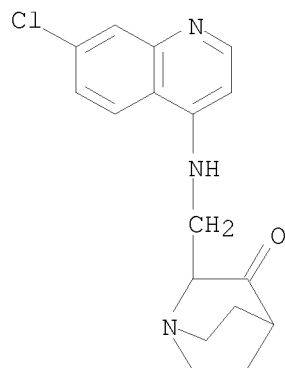
IT 21566-68-7P 22776-50-7P 22776-52-9P

22950-03-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

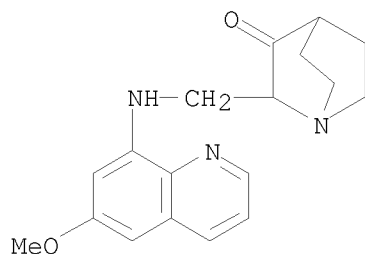
RN 21566-68-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[(7-chloro-4-quinolinyl)amino]methyl]-
(CA INDEX NAME)

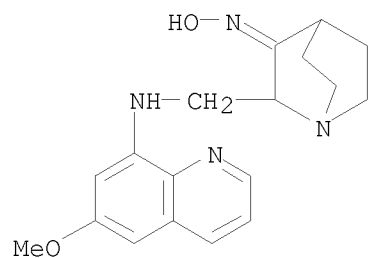


RN 22776-50-7 CAPLUS

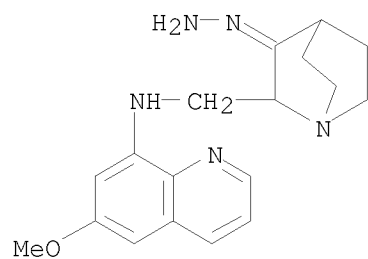
CN 3-Quinuclidinone, 2-[[[(6-methoxy-8-quinolyl)amino]methyl]- (8CI) (CA
INDEX NAME)



RN 22776-52-9 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, oxime (8CI)
(CA INDEX NAME)



RN 22950-03-4 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, hydrazone
(8CI) (CA INDEX NAME)



L9 ANSWER 151 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:459119 CAPLUS
DOCUMENT NUMBER: 69:59119
ORIGINAL REFERENCE NO.: 69:11047a,11050a
TITLE: 2-Methylene-3-quinuclidinone
INVENTOR(S): Biel, John H.; Hopps, Harvey B.; Bader, Henryk
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3384641	A	19680521	US 1967-668941	19670919
PRIORITY APPLN. INFO.:			US 1967-668941	A 19670919

GI For diagram(s), see printed CA Issue.

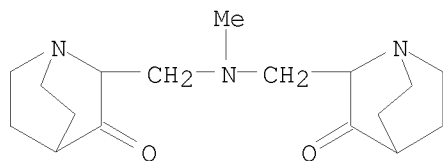
AB The title compound (I) is prepared by heating the Mannich reaction product of 3-quinuclidinone (II), Me₂NH, and HCHO; it is used to sep. tertiary from primary and secondary amines. Thus, 200 g. II, 270 g. 40% Me₂NH, 194.8 g. 37% HCHO, 250 ml. EtOH, and 100 ml. water was refluxed 1 hr., held 17 hrs. at 70°, and worked up to give 203 g. I, b₇ 91-2°, n_D 1.5110; HCl salt m. 284-8°. A mixture of pyridine and piperidine was separated by distillation in the presence of I. The piperidine distilled only after its reaction product with I decomposed. MeNH₂ was also purified by adding 13.7 g. I in 20 ml. MeOH to 3.88 g. 40% aqueous MeNH₂ and heating 1 hr. at 50° to give 11 g. 2,α'-methyliminobis(2-methyl-3-quinuclidinone) monohydrate, m. 90-2°, which was decomposed by gentle heating to pure MeNH₂, leaving I as a residue.

IT 19576-25-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19576-25-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis-
(9CI) (CA INDEX NAME)



L9 ANSWER 152 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:427579 CAPLUS

DOCUMENT NUMBER: 69:27579

ORIGINAL REFERENCE NO.: 69:5155a,5158a

TITLE: Synthetic quinine analogs. I. Synthesis and some chemical transformations of 6'-methoxy-7-oxo-8-rubene

AUTHOR(S): Bender, D. R.; Coffen, D. L.

CORPORATE SOURCE: Univ. of Colorado, Boulder, CO, USA

SOURCE: Journal of Organic Chemistry (1968), 33(6), 2504-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

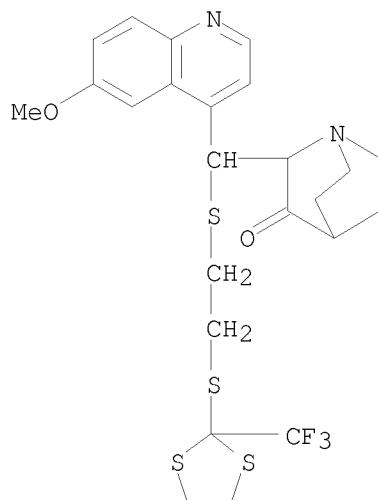
AB NaOEt-catalyzed condensation of 6-methoxyquinoline-4-carboxaldehyde with 3-quinuclidinone produces 6'-methoxy-7-oxo-8-rubene (I) in high yield. Of the 2 possible geometrical isomers, only that with the ketone function trans to the quinoline ring is formed. Reduction of I affords an allylic alc. whose p-nitrobenzoate is completely isomerized to the opposite geometrical isomer in refluxing HOAc. I is not ketalized by 1,2-ethanedithiol in refluxing F3CCO2H involving 1 mol. of ketone, 2 of 1,2-ethanedithiol, and 1 of F3CCO2H. A by-product of the reaction results from the condensation of 3 mols. of 1,2-ethanedithiol with 2 of F3CCO2H. Pyrazoline derivs. of I resulting from 1,3-dipolar addition of CH2N2 and condensation with hydrazine are described. 24 references.

IT 16526-37-7P

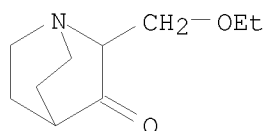
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16526-37-7 CAPLUS

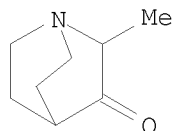
CN Orthoacetic acid, trifluorotrithio-, cyclic ethylene ester, ester with 2-[[[(2-mercaptoethyl)thio](6-methoxy-4-quinolyl)methyl]-3-quinuclidinone, (±)- (8CI) (CA INDEX NAME)



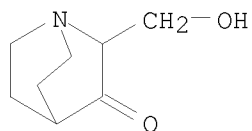
L9 ANSWER 153 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1966:84473 CAPLUS
 DOCUMENT NUMBER: 64:84473
 ORIGINAL REFERENCE NO.: 64:15837a-b
 TITLE: Systems with bridgehead nitrogen. β -Ketols of the
 1-azabicyclo[2.2.2]octane series
 AUTHOR(S): Nielsen, Arnold T.
 CORPORATE SOURCE: Chem. Div., U.S. Naval Ordnance Test Sta., China Lake,
 CA
 SOURCE: Journal of Organic Chemistry (1966), 31(4), 1053-9
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The prepn. and chemical behavior of the β -ketols incorporating the
 1-azabicyclo [2.2.2] octane ring are described. Three different
 structural types are represented in this study. Methylation of
 3-quinuclidinone with excess formaldehyde (potassium carbonate catalyst
 under appropriate conditions) led to 2,2-bismethylol-3-quinuclidinone (I)
 or 2-methylene-3-quinuclidinone (II). 2-Methylol-3-quinuclidinone (III)
 was prepared by hydration of II cation. Starting with 4-acetylpiperidine
 and its N-benzyl derivative, syntheses of 4-hydroxymethyl-3-quinuclidinone
 (IV) and 4-acetyl-3-quinuclidinol (V) were achieved. The bridgehead IV
 was extremely stable whereas V underwent facile retrograde aldolization in
 basic media. I readily loses one methylol group in base leading to III,
 which dehydrates with extreme ease rather than undergo demethylation.
 IT 5291-13-4P, 3-Quinuclidinone, 2-(ethoxymethyl)- 5291-14-5P
 , 3-Quinuclidinone, 2-methyl- 5291-27-0P, 3-Quinuclidinone,
 2-(hydroxymethyl)- 5291-32-7P, 3-Quinuclidinone,
 2-(hydroxymethyl)-2-(methoxymethyl)- 5291-33-8P,
 3-Quinuclidinone, 2-(ethoxymethyl)-, picrate 5291-34-9P,
 3-Quinuclidinone, 2-methyl-, picrate 5291-35-0P,
 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 5291-13-4 CAPLUS
 CN 3-Quinuclidinone, 2-(ethoxymethyl)- (7CI, 8CI) (CA INDEX NAME)



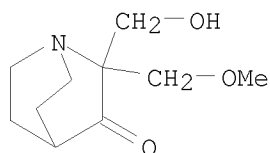
RN 5291-14-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)



RN 5291-27-0 CAPLUS
 CN 3-Quinuclidinone, 2-(hydroxymethyl)- (7CI, 8CI) (CA INDEX NAME)



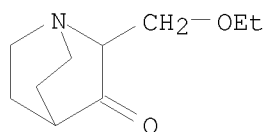
RN 5291-32-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)- (CA INDEX NAME)



RN 5291-33-8 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(ethoxymethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

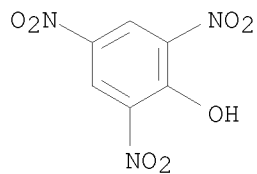
CM 1

CRN 5291-13-4
 CMF C10 H17 N O2



CM 2

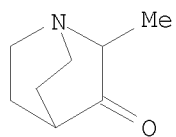
CRN 88-89-1
 CMF C6 H3 N3 O7



RN 5291-34-9 CAPLUS
 CN 3-Quinuclidinone, 2-methyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

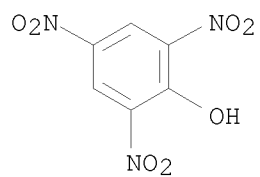
CRN 5291-14-5
 CMF C8 H13 N O



CM 2

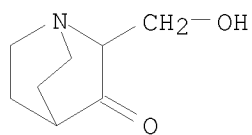
CRN 88-89-1

CMF C6 H3 N3 O7



RN 5291-35-0 CAPLUS

CN 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

ACCESSION NUMBER: 1964:9663 CAPLUS
 DOCUMENT NUMBER: 60:9663
 ORIGINAL REFERENCE NO.: 60:1697e-h,1698a-h,1699a
 TITLE: Quinuclidine series. VII. Solvolysis of
 2-(α -chlorobenzyl)quinuclidine. The
 heterocinchonine rearrangement
 AUTHOR(S): Braschler, V.; Grob, C. A.; Kaiser, A.
 CORPORATE SOURCE: Univ. Basel, Switz.
 SOURCE: Helvetica Chimica Acta (1963), 46(7), 2646-58
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 60:9663

AB cf. CA 53, 4278e. The rate and the products of the hydrolysis of
 2-(α -chlorobenzyl)quinuclidine (I) do not provide evidence for the
 participation of the quinuclidine N in the ionization step, and no product
 derived from a heterocinchonine rearrangement could be isolated.
 2-Benzyl-2-dehydroquinuclidine (II) and 2-benzylidenequinuclidine (III)
 possess abnormal spectral and chemical properties ascribable to steric
 inhibition of the vinylamine-type mesomerism. Et isonicotinate (151 g.)
 and 167 g. BrCH₂CO₂Et in 500 cc. EtOH kept at room temperature overnight,
 refluxed 4 hrs., hydrogenated 0.5-1 hr. at 90°/100 atmospheric over 15 g.
 10% Pd-C, filtered, the filtrate evaporated at 50-60°, the semicryst.
 residue treated with cooling and shaking with 500 cc. cold H₂O, 500 cc.
 CHCl₃, and 150 g. K₂CO₃ in 250 cc. H₂O, and the organic layer worked up
 yielded 180-90° 4-carbethoxy-1-carbethoxymethylpiperidine (IV),
 b_{0.2} 111-13°, n_{20D} 1.4585, d₁₅₁₅ 1.057. IV (100 g.) in 250 cc.
 absolute MePh added dropwise during 1.5 hrs. to KOEt (from 39.096 g. K and 60
 cc. EtOH in 162 cc. dry MePh) the mixture stirred 4 hrs. at 130°,
 cooled, the MePh decanted, extracted with 50 cc. H₂O, the residue dissolved in
 300 cc. EtOH, combined with the aqueous extract, the solution adjusted with
 100 cc.
 10N HCl with cooling and stirring to pH 7 below 30°, cooled to
 0°, filtered, the filtrate adjusted with about 2 cc. AcOH to pH 4,
 concentrated to about 200 cc., treated with 20 cc. saturated aqueous KHCO₃,
 and extracted
 with CHCl₃ yielded 57 g. 2-carbethoxy-3-quinuclidone (V), b_{0.02}
 98-103°, m. 116-20° (absolute EtOH-Et₂O). V (20 g.), 80 cc. dry
 Et₃N, and 100 cc. absolute EtOH hydrogenated over about 5 g. Raney Ni under
 ambient conditions yielded 10.9 g. 2-carbethoxy-3-hydroxyquinuclidine (VI)
 isomer A (VII), m. 147-8° (Me₂CO), (sublimation); the filtrate was
 evaporated and the cryst, residue (9 g.) chromatographed on 200 g. Al₂O₃ to
 give 2.34 g. VII, 4.7 g. isomer mixture, m. 72-105°, and 1.98 g. VI
 isomer B, m. 100-2°; VI.MeI, m. 175-8° (decomposition)
 (EtOH-Et₂O). VI (21.1 g.) and 150 cc. Ac₂O refluxed 6 hrs., the mixture
 evaporated, the oily residue partitioned between 200 cc. Et₂O and 50 cc. 2N
 HCl, the Et₂O phase extracted with 2N HCl, the combined aqueous solns.
 saturated with
 solid K₂CO₃, and extracted with Et₂O gave 14.4 g. 2-carbethoxy-2-
 dehydroquinuclidine (VIII), b₁₂ 128-30°, n_{25D} 1.4955, and 1.1 g.
 acetate of VI, b₁₂ 130-63°. VIII (12.7 g.) in 65 cc. EtOH
 hydrogenated 1 hr. over 600 mg. 10% Pd-C under ambient conditions yielded
 12.1 g. 2-carbethoxyquinuclidine, b₁₁ 119-20°, n_{25D} 1.4752, b₁₁
 119-20°; picrate m. 120° (EtOH). VIII (10 g.) and 150 cc.
 saturated NH₃-MeOH heated 15 hrs. at 100° in an autoclave gave 7.5 g.
 2-CONH₂ analog (IX) of VIII, m. 178-81° (Me₂CO). IX (5.45 g.) in
 50 cc. MeOH and 25 cc. H₂O hydrogenated 2 hrs. over Raney Ni W-7 under
 ambient conditions yielded 4.9 g. 2-carbamoylquinuclidine (X), m.
 148-9° (Me₂CO). 2-Carbethoxyquinuclidine (1.2 g.) and 10 cc.
 NH₃-MeOH (saturated at 20°) heated 48 hrs. at 100° in a sealed
 tube gave 0.81 g. X, m. 145-6° (Me₂CO). IX (5.6 g.) in 45 cc. Et₃N

and 25 cc. CHCl₃ mixed with 10.5 g. P₂O₅ g. and 50 g. sand, refluxed 30 hrs., cooled, the supernate decanted, the residual oil washed with Et₂O, the residue treated with saturated aqueous K₂CO₃ and extracted with Et₂O, and the combined washings, and decantate worked up yielded 0.92 g. unreacted IX, m. 177-80°; the mother liquor distilled gave 2 g. 2-CN analog of VIII, b₁₁ 120-3°, n_D 24.5D 1.5068. X (12.2 g.), 22.5 g. P₂O₅, and 50 g. sand refluxed 26 hrs. with 90 cc. dry Et₃N and 60 cc. dry CHCl₃ and similarly worked up yielded 8.25 g. 2-cyanoquinuclidine (XI), b₁₃ 105-21°; picrate m. 216-26° (decomposition) (Me₂CO-EtOH); XI.MeI m. 247-50° (decomposition) (absolute EtOH). X (9.4 g.), 50 cc. Ac₂O, and 50 cc. Et₃N refluxed 10 hrs. yielded 4 g. XI, b₁₃ 105-21°. XI (17.4 g.) in 300 cc. dry C₆H₆ added dropwise during 1 hr. to PhMgBr from 6.5 g. Mg, 40.2 g. PhBr, and 170 cc. dry Et₂O and the mixture refluxed 4 hrs. yielded 20.9 g. 2-benzoylquinuclidine (XII), m. 88-9.5° (Et₂O); the residue from the mother liquor sublimed at 120-40°/11 mm. gave 1.35 g. XII, m. 86-9°; picrate m. 174-8° (EtOH); methiodide m. 196-8° (Me₂CO). XII (1 g.) and 0.335 g. NH₂OH.HCl in 20 cc. MeOH refluxed 24 hrs. yielded the oxime of XII, m. 194-5.5° with sublimation (AcOEt); picrate m. 194-8° with sublimation (EtOH) XII (4.0 g.) in 50 cc. dry Et₂O added dropwise during 10 min. with stirring to 0.5 g. LiAlH₄ in 50 cc. dry Et₂O, the mixture refluxed 3 hrs., stirred 12 hrs. at room temperature, and decomposed with 30 cc. iced H₂O and 25 cc. concentrated HCl yielded the mixed isomeric 2-(α-hydroxybenzyl)quinuclidine (XIII), which-recrystd. repeatedly from Me₂CO gave 800 mg. isomer A (XIIIa), m. 142-4° [picrate m. 191-4° (EtOH)]; the residue (2.9 g.) from the mother liquor chromatographed on 60 g. Al₂O₃ gave the isomer B (XIIIb), m. 75-6.5° (petr. ether) [picrate m. 183-6° (EtOH)]. XIII (3 g.) and 30 cc. SOCl₂ refluxed 12 hrs., the mixture evaporated, and the residue evaporated twice with C₆H₆ and fractionally recrystd. from absolute EtOH yielded I.HCl isomer A (Ia.HCl), m. 238-40° (absolute EtOH-Et₂O) [picrate m. 183-6° (EtOH)], and I.HCl isomer B (Ib.HCl), m. 245-9.5° (decomposition) [picrate m. 173-4° (EtOH)]. Ia (1.89 g.) in 5 cc. absolute EtOH refluxed 3 hrs. with 3.5 g. KOH in 20 cc. absolute EtOH yielded 1.39 g. III isomer A (IIIa), b₁₂ 168-70° [picrate m. 149-50° and then 167-9° (EtOH)]. Ib (500 mg.) and 1 g. KOH in 10 cc. absolute EtOH refluxed 14 hrs. yielded 394 mg. oily III isomer B (IIIb) [picrate m. 162-3° and then 180-1° (iso-PrOH-Me₂CO)]. Quinuclidone-HCl (8.5 g.) and 15 g. BzH refluxed 10 hrs. with 7.5 g. KOH in 150 cc. absolute EtOH yielded 8.07 g. 2-benzylidene-3-quinuclidone (XIV), m. 134-7° (MeOH) [picrate m. 180-4° (EtOH)]. XIV (11.05 g.) in 300 cc. MeOH hydrogenated under ambient conditions over Raney Ni, and the product fractionally recrystd. from Me₂COMeOH yielded 7.7 g. 2-benzyl-3-hydroxyquinuclidine isomer A (XVa), m. 157-8° [picrate m. 128-32° (iso-PrOH); HCl salt m. 203-7° (MeOH-Me₂CO-Et₂O)]; the residue (2.85 g.) from the mother liquor chromatographed on 60 g. Al₂O₃ yielded 1.5 g. XV isomer B (XVb), m. 129-33° (Me₂CO) [picrate, m. 159-62° (iso-PrOH)], and 1.3 g. mixed XVa and XVb. XVa (5 g.) and 50 cc. SOCl₂ refluxed 70 hrs. gave 2 g. II, b₀.005 62°, n_D 23D 1.5485, which solidified at -15° [picrate m. 200-5° (Me₂CO)], and 1.9 g. 2-benzyl-3-chloroquinuclidine, b₀.005 73-5°, picrate m. 184-7° with a change to plates and then m. 201-3° (iso-PrOH). I.HCl (500 mg.) in 25 cc. EtOH hydrogenated about 2 hrs. over 50 mg. 10% Pd-C yielded 2-benzylquinuclidine-HCl (XVI.HCl), m. 268-9° (EtOH-Et₂O) (with sublimation); picrate m. 184-6° (EtOH). IIIa or IIIb (200 mg.) in EtOH hydrogenated over Pd-C yielded XVI isolated as picrate, m. 183-6° (EtOH); XVI.HCl m. 270-2° (EtOH-Et₂O). II (260 mg.) in 5 cc. EtOH hydrogenated over Raney Ni yielded XVI isolated as the picrate, m. 180.5-3.5° (iso-PrOH). I.HCl (2.0017 g.), 8 cc. N NaOH, 32.4 cc. H₂O, and 32.4 cc. Me₂CO heated 24 hrs. at 68°, cooled, acidified with 2N HCl, concentrated to 20 cc. at 45°, basified

with saturated aqueous K₂CO₃, and extracted with CHCl₃, and the residue from the extract

chromatographed on Al₂O₃ yielded 100 mg. substance which gave the picrate of IIIa, m. 145-50° and then 167-9° (EtOH), 110 mg. oil which yielded the picrate of XIII, m. 278-81° (EtOH) [free base m. 72-8° (petr. ether)], and 110 mg. oily C₁₃H₁₇NO (XVII); picrate m. 186-8° (EtOH); HCl salt m. 157-8° (decomposition) (iso-PrOH-Et₂O). I.HCl (4 g.), 5.94 g. Et₃N, 40 cc. H₂O, and 40 cc. Me₂CO refluxed 42 hrs., cooled, acidified with 2N HCl, concentrated to 30 cc., basified with saturated aqueous K₂CO₃, and extracted with Et₂O, and the oily

residue

(3.1 g.) from the extract chromatographed on Al₂O₃ gave 103 mg. III, 210 mg. XIII, and 56 mg. XVII. I.HCl (1.3 g.) treated in the usual manner with K₂CO₃, the free base stirred 24 hrs. at room temperature in 100 cc. 60% aqueous Me₂CO with 2 equivs. Ag₂O, refluxed 24 hrs., filtered through Celite, acidified with 2N HCl, concentrated to 20 cc., basified with saturated aqueous

K₂CO₃,

and extracted with CHCl₃, and the oily residue from the extract distilled gave

510

mg. yellow oil, b_{0.01} 90-110°, which chromatographed on Al₂O₃ yielded 147 mg. III, 89 mg. XIII, and 155 mg. oily XVII.

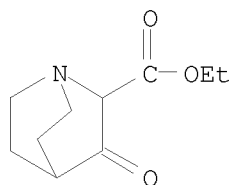
IT 34286-16-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester

RL: PREP (Preparation)

(preparation of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



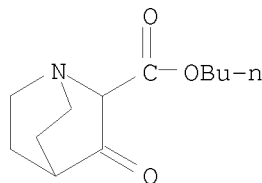
L9 ANSWER 155 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:410798 CAPLUS
DOCUMENT NUMBER: 57:10798
ORIGINAL REFERENCE NO.: 57:2192e-i
TITLE: Synthesis of 2,3-quinuclidinedicarboxylic acid
AUTHOR(S): Mikhлина, E. E.; Rubtsov, M. V.; Vorob'eva, V. Ya.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem.-Pharm. Res. Inst.,
Moscow
SOURCE: Zhurnal Obshchei Khimii (1961), 31, 3251-5
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10798

AB cf. CA 54, 9945i. Azeotropic removal of H₂O from 69.3 g. KOH, 11. BuOH, and 100 ml. MePh, evaporation of the residue, and treatment with 120 g. 1-carbethoxymethyl-4-carbethoxypiperidine 5 hr. in MePh gave a viscous mass containing K salt of the enol of Bu 3-oxoquinuclidine-2-carboxylate, which treated with 10% AcOH followed by K₂CO₃ gave 43.5% Bu 3-oxo-quinuclidine-2-carboxylate, b_{0.6} 137° m. 88°; HCl salt m. 163°. The latter treated with aqueous KCN at 5° gave 68.5% cyanohydrin, m. 107°. Similarly was prepared the cyanohydrin of the Et ester, m. 124-5°. This refluxed 25 hrs. with AcOH-HCl then esterified with EtOH-HCl gave some 3-quinuclidone, separated by sublimation, and 30% di-Et 3-hydroxyquinuclidine-2,3-dicarboxylate (I), b_{1.2} 142°, m. 104-5°, also formed from the corresponding Bu ester cyanohydrin. Refluxing the di-Et ester with 1:1 HCl 5 hrs. gave 65% 3-hydroxyquinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 126°. I with SOCl₂ 30 hrs. followed by aqueous K₂CO₃ gave 74.5% di-Et Δ²-dehydroquinuclidine-2,3-dicarboxylate, b_{0.5} 130°; HCl salt m. 148.5°. This refluxed 5 hrs. with 1:1 HCl gave 99% Δ²-dehydroquinuclidine-2,3-dicarboxylic acid, decomposed at 240°; HCl salt, hygroscopic crystals, hydrolyzed by H₂O. Hydrogenation over Pt gave quinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 138°, which refluxed 5 hrs. with EtOH-HCl gave the di-Et ester (II), b_{0.4} 115°, which with LiAlH₄ gave 58% 2,3-bis(hydroxymethyl)quinuclidine, b_{0.3} 150°; HCl salt, hygroscopic crystals. This and AcCl in refluxing CHCl₃ 5 hrs. gave 70% diacetate, b_{0.6} 138-40°. II kept 7 days in H₂O gave 83.5% 3-carbethoxyquinuclidine-2-carboxylic acid, decomposed at 188-9°.

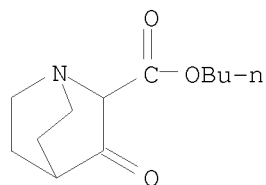
IT 91554-81-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride 91554-82-4P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester
RL: PREP (Preparation)
(preparation of)

RN 91554-81-3 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride (7CI)
(CA INDEX NAME)



RN 91554-82-4 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester (7CI) (CA INDEX NAME)



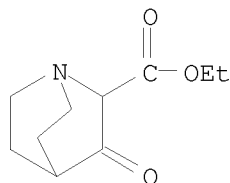
L9 ANSWER 156 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1960:50470 CAPLUS
DOCUMENT NUMBER: 54:50470
ORIGINAL REFERENCE NO.: 54:9945i,9946a-c
TITLE: Amino acids of the quinuclidine series
AUTHOR(S): Yakhontov, L. N.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Research
Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 2343-8
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:50470

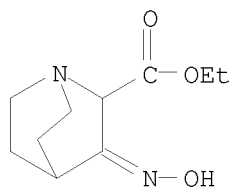
AB Keeping 1.1 g. 2-formylquinuclidine and 0.9 g. EtO₂CCH₂CN in 3 ml. pyridine with 5 drops piperidine 10 days gave a precipitate of 97.2% Et β -(2-quinuclidyl)- α -cyano-acrylate, m. 139.5-41° (picrate, m. 130.5-10°), which hydrogenated over Pt to α -aminomethyl- β -(2-quinuclidyl)propionic acid, isolated as dipicrate, decomposing 125°; the acid was isolated after the original reaction mixture was hydrogenated and then refluxed with concentrated HCl. Keeping an aqueous solution of Na salt of enol form of Et β -(2-quinuclidyl)- β -oxopropionate 1 day gave Na β -(2-quinuclidyl)- β -oxopropionate, decomposing 240°; this with HONH₂ gave 93% β -(2-quinuclidyl)- β -oxopropionic acid oxime, an oil; di-HCl salt, decompose 284°; picrate, m. 167-70°. Hydrogenation of the oxime over Pt gave 78% β -(2-quinuclidyl)- β -aminopropionic acid isolated as di-HCl salt, decomposing 283°. To KOEt in dry MePh was added at 120° 1-carbethoxymethylisonipecotinic acid, the whole was refluxed 5 hrs., cooled, the precipitated K salt of Et 3-oxo-2-quinuclidinecarboxylate was separated and treated with dilute AcOH, yielding

75% Et 3-oxo-2-quinuclidinecarboxylate, m. 109-10°. This with HONH₂.HCl in EtOH gave 80% corresponding oxime, isolated as HCl salt, decomposing 196°. This, hydrogenated over Pt to 99.4% Et 3-amino-2-quinuclidinecarboxylate di-HCl salt, decomposing 185°. This heated with concentrated HCl 6 hrs. gave 91% 3-amino 2-quinuclidinecarboxylic acid di-HCl salt, decomposing 242°.

IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

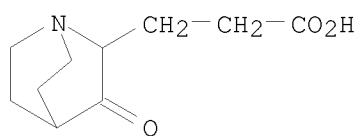


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)

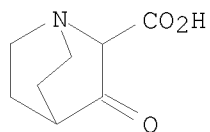


● HCl

RN 117342-57-1 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 857019-15-9, 2-Quinuclidinecarboxylic acid, 3-oxo-
 (derivs.)
 RN 857019-15-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo- (CA INDEX NAME)



ACCESSION NUMBER: 1960:50469 CAPLUS
 DOCUMENT NUMBER: 54:50469
 ORIGINAL REFERENCE NO.: 54:9945d-i
 TITLE: Phenanthryl substituted barbiturates
 AUTHOR(S): Giannini, M.; Fedi, M.; Russo, F.
 CORPORATE SOURCE: Lab. chim. farm. A. Menarini, Florence
 SOURCE: Bollettino Chimico Farmaceutico (1959), 98, 714-21
 CODEN: BCFAAI; ISSN: 0006-6648
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Refluxing 2.26 g. 9-(chloromethyl)phenanthrene (I) with 62 ml. PrOH, adding 1.42 g. 5-methylbarbituric acid and 0.8 g. HCO₂Na in 7 ml. H₂O, refluxing 7 hrs., distilling the PrOH to a small volume, mixing the residue with

100 ml. H₂O, filtering, and washing with C₆H₆ until the product was colorless, gave 0.8 g. 5-(9-phenanthrylmethyl)-5-methylbarbituric acid, m. 233-5° (MePh). Refluxing 2.26 g. I in 62 ml. PrOH with 1.56 g. ethylbarbituric acid and 0.8 g. AcONa in 7 ml. H₂O for 5 hrs., distilling the solvent, taking up with 100 ml. H₂O, allowing to stand, and washing with C₆H₆ gave 1.2 g. 5-(9-phenanthrylmethyl)-5-ethylbarbituric acid (II), m. 237-8° (xylene). By an analogous procedure there were prepared the following analogs of II: 5-Pr, m. 240° (MePh); 5-Bu, m. 245-8° (MePh and C₆H₆); 5-allyl, m. 228-30° (xylene).

Adding to 6.3 g. K₂Cr₂O₇ in 19 g. H₂SO₄ and 31 ml. H₂O at water bath temperature

2 g. I, adding later 6.3 g. K₂Cr₂O₇, heating to boiling, cooling, diluting with H₂O, washing thoroughly, digesting the solid with NaHSO₃ solution at 50-60°, precipitating the phenanthrenequinone with dilute H₂SO₄ and subliming gave the pure quinone, m. 204°. Treating this quinone in EtOH with o-phenylenediamine gave the corresponding phenazine, m. 217°.

Refluxing 2 g. II 48 hrs. with 20 ml. 25% NaOH solution and 20 ml. EtOH, diluting with H₂O, acidifying with 10% H₂SO₄, keeping for crystallization, filtering,

dissolving with NaHCO₃ solution, precipitating with H₂SO₄, dissolving in Et₂O, and

precipitating with petr. ether gave 0.5 g. ethyl-(9-phenanthrylmethyl)malonic acid, m. 152-4° (decomposition). Refluxing 2.26 g. I with 1.58 g. 5-methyl-2-thiobarbituric acid in 60 ml. PrOH to dissoln., adding 0.8 g. NaOAc in 7 ml. H₂O, refluxing 1 hr., distilling the PrOH to a small volume, adding 100 ml. H₂O, washing the crystals with C₆H₆, dissolving repeatedly in NaOH and precipitating with HCl gave 2.15 g.

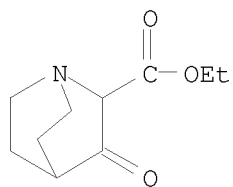
5-(9-phenanthrylmethyl)-5-methyl-2-thiobarbituric acid, m. 280-2°. By an analogous procedure with 0.1 mole material were prepared 3.4 g. 5-Et analog., 250-3° (xylene), 2.5 g. Pr analog. m. 230-1° (xylene), 0.8 g. Bu analog, m. 210° (xylene), and 0.8 g. allyl analog m. 185-9° (MePh). Dissolving 7.4 g. Na in 135 anhydrous EtOH, adding 8.5 g. thiourea and 20 g. di-Et allylmalonate, refluxing 4 hrs., dissolving the precipitate in a min. volume of H₂O, and precipitating with HCl gave 3.52 g. 5-allyl-2-thiobarbituric acid, m. 120-2° (xylene). By the same method was prepared from 11.5 g. thiourea and 25 g. di-Et propylmalonate 5.37 g. 5-propyl-2-thiobarbituric acid, m. 163-5° (H₂O).

IT 34286-16-3 110056-51-4 117342-57-1

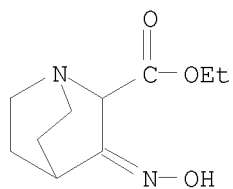
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

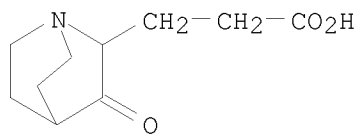


RN 110056-51-4 CAPLUS
 CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride
 (6CI) (CA INDEX NAME)



● HCl

RN 117342-57-1 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)

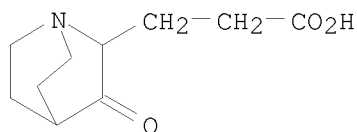


ACCESSION NUMBER: 1959:122172 CAPLUS
DOCUMENT NUMBER: 53:122172
ORIGINAL REFERENCE NO.: 53:21953f-i,21954a-c
TITLE: Cyanoethylation of 3-quinuclidinone
AUTHOR(S): Mikhлина, E. E.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research
Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 118-24
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Na (24 g.) in 100 ml. MePh and 36 ml. absolute EtOH heated to 120-5°, treated over 1 hr. with 60 g. 1-carbethoxymethyl-4-carbethoxypiperidine in 150 ml. MePh, refluxed 5 hrs., treated with 200 ml. concentrated HCl, the mixture stirred 0.5 hr., the organic layer separated, reextd. with 200 ml. concentrated HCl twice, the acid exts. combined, refluxed 15 hrs., decolorized, and the residue evaporated, treated with 50% KOH, and extracted with C₆H₆ gave 84.6% 3-quinuclidinone, m. 136-8°; picrate, m. 210°. This (25 g.) in 115 ml. dry dioxane and 3.8 ml. 30% KOH in MeOH heated to 60°, treated over 0.5 hr. with 90 ml. CH₂:CHCN, stirred 4 hrs. at 60°, the amorphous polymer filtered off, the filtrate freed of dioxane in vacuo, the residue treated with 100 ml. C₆H₆, extracted with 50 ml. 10% HCl, and the acid extract treated with K₂CO₃, and extracted with C₆H₆ yielded on distillation 14.3 g. 3-quinuclidinone. The distillation residue with 20 ml. absolute EtOH and 1 ml. dry C₆H₆ yielded 4 g. 3-oxo-2,2-bis(2-cyanoethyl)quinuclidine (Ia), m. 120-2° (EtOH); the mother liquor gave 0.7 g. 3-oxo-2-(2-cyanoethyl)quinuclidine (I), b_{0.3} 121-2°. The same products were formed in Me₃COH with MeOH-KOH catalyst. Refluxing I with HCl-AcOH 20 hrs. gave crude 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, which, heated 3 hrs. with 9% alc.-dry HCl gave 60.6% 3-oxo-2-(2-carbethoxyethyl)quinuclidine (II), b_{0.4} 136-8°, after the usual treatment of the mixture with K₂CO₃; the ester refluxed 4 hrs. with 17% HCl gave 96.5% 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, decompose 191-3° (EtOH). Heating 0.3 g. II and 1.8 ml. N₂H₄.H₂O with 0.4 g. Na in 9 ml. absolute EtOH in a sealed tube 14 hrs. at 170-80°, distilling the EtOH, refluxing the residue 4 hrs. with 10 ml. H₂O, acidifying with HCl, evaporating, heating the residue with 10 ml. 10% alc. HCl 3 hrs., distilling the EtOH, treating the residue with K₂CO₃, and extracting with Et₂O gave 0.17 g. 2-(2-carbethoxyethyl)quinuclidine, b_{0.2} 90-2°, which, refluxed 4 hrs. with 17% HCl, gave 0.06 g. 2-(2-carboxyethyl)quinuclidine HCl salt, decompose 216.5-17.5°. Reduction of II with LiAlH₄ in Et₂O gave 56.7% 3-hydroxy-2-(3-hydroxypropyl)quinuclidine, b_{0.4} 163-5°; HCl salt, m. 132-3°. Refluxing Ia with AcOH-concentrated HCl 17 hrs. gave 92% 3-oxo-2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 245° (90% EtOH). This refluxed 4 hrs. with 9% alc. HCl gave 63.6% 3-oxo-2,2-bis(2-carbethoxyethyl)quinuclidine (III), b₁ 190°, m. 58-61°; HCl salt, m. 169-71° (EtOH). Reductions of III with LiAlH₄ in Et₂O gave 85% 3-hydroxy-2,2-bis(3-hydroxypropyl)quinuclidine, hygroscopic crystals; HCl salt, m. 221-3° (EtOH). Keeping 0.35 g. III with 0.6 ml. N₂H₄.H₂O in 2 ml. absolute EtOH 8 days gave 0.2 g. III dihydrazide, hygroscopic solid yielding a picrate, decompose 168°. Heating III with N₂H₄.H₂O in EtOH-EtONa, as above, 14 hrs. at 160-70° gave 50% 2,2-bis(2-carbethoxyethyl)quinuclidine, b_{0.2} 175-80°, which, refluxed 4 hrs. with 17% HCl, gave 30% 2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 215-18° (Me₂CO-EtOH). Heating 1.2 g. LiAlH₄, 1 g. Ia, 45 ml. C₆H₆, and 20 ml. absolute Et₂O 40 hrs. at 65-70°, adding 3 ml. H₂O, separating the inorg.

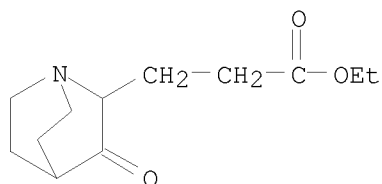
salts, washing these with dry pyridine, and evaporating the filtrate gave 59.6% 3-hydroxy-2,2-bis-(2-cyanoethyl)quinuclidine, m. 179-80° (absolute EtOH).

IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 75208-48-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI)
(CA INDEX NAME)



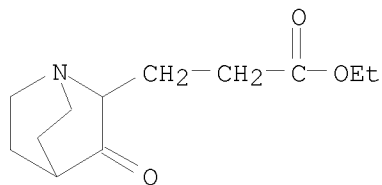
● HCl

RN 105339-98-8 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI)
(CA INDEX NAME)

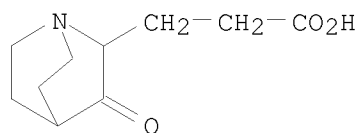


● HCl

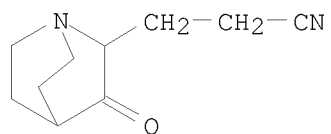
RN 105339-99-9 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



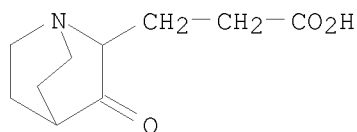
IT 117342-57-1, 2-Quinuclidinepropionic acid, 3-oxo-
(derivs.)
RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 99169-54-7P, 2-Quinuclidinepropionitrile, 3-oxo-
 RL: PREP (Preparation)
 (preparation of)
 RN 99169-54-7 CAPLUS
 CN 2-Quinuclidinepropionitrile, 3-oxo- (6CI) (CA INDEX NAME)

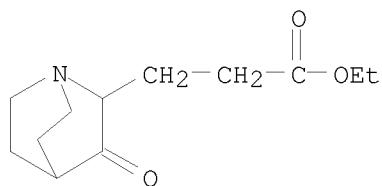


L9 ANSWER 159 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1959:122171 CAPLUS
 DOCUMENT NUMBER: 53:122171
 ORIGINAL REFERENCE NO.: 53:21953e-f
 TITLE: Syntheses in the allo-lupinane series. IV. An
 alternative synthesis of 4-hydroxymethylquinolizidine
 AUTHOR(S): Lukes, R.; Vesely, Z.
 CORPORATE SOURCE: Vysoka skola chem. technol., Prague
 SOURCE: Collection of Czechoslovak Chemical Communications
 (1959), 24, 2318-23
 CODEN: CCCCAK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB See C.A. 53, 368f.
 IT 75208-48-9 105339-98-8 105339-99-9
 (Derived from data in the 6th Collective Formula Index (1957-1961))
 RN 75208-48-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI)
 (CA INDEX NAME)



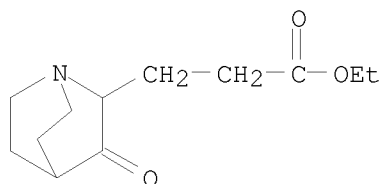
● HCl

RN 105339-98-8 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI)
 (CA INDEX NAME)



● HCl

RN 105339-99-9 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)




```
=> s l9 and cancer
      362087 CANCER
      53250  CANCERS
      375482 CANCER
              (CANCER OR CANCERS)
L10           4 L9 AND CANCER

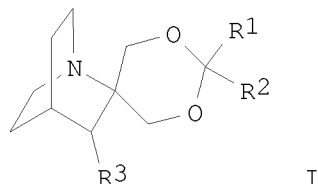
=> d ibib abs hitstr tot
```

L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:590850 CAPLUS
DOCUMENT NUMBER: 147:2004
TITLE: Quinuclidinone derivatives as anticancer agents
INVENTOR(S): Bergmeier, Stephen C.; Evans, Susan C.
PATENT ASSIGNEE(S): Ohio University, USA
SOURCE: PCT Int. Appl., 21pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007062030	A2	20070531	WO 2006-US45045	20061121
WO 2007062030	A3	20080124		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRIORITY APPLN. INFO.: US 2005-738673P P 20051121
OTHER SOURCE(S): MARPAT 147:2004
GI

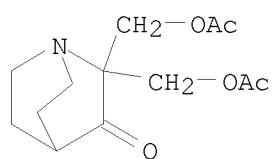


AB The invention discloses compds. I (R1, R2 = H, halo, alkyl, cycloalkyl, haloalkyl, aryl, etc.; R3 = O, OH), as well as derivs., metabolites, and prodrugs thereof. Also provided are methods for preparing the quinuclidinone analogs. Further provided are methods for treating, preventing, or delaying the onset of a cancer in a subject in need of such treatment by administering a an effective amount of I, or a derivative, metabolite, or prodrug thereof, to a subject diagnosed with cancer or at risk of developing cancer.

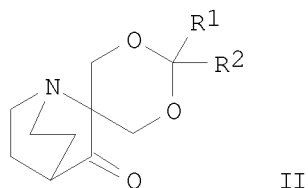
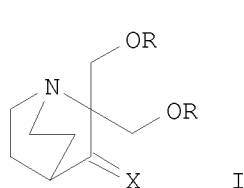
IT 865293-04-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(quinuclidinone derivative anticancer agents)

RN 865293-04-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)

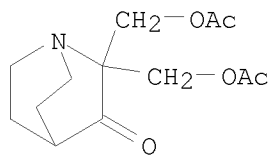


ACCESSION NUMBER: 2006:87882 CAPLUS
 DOCUMENT NUMBER: 144:331585
 TITLE: Structure-activity studies of quinuclidinone analogs as anti-proliferative agents in lung cancer cell lines
 AUTHOR(S): Malki, Ahmed; Pulipaka, Aravinda B.; Evans, Susan C.; Bergmeier, Stephen C.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, Ohio University, Athens, OH, 45701, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(5), 1156-1159
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:331585
 GI



AB Novel quinuclidinone analogs, such as I [R = H, COMe, X = :O; R = H, X = H, OH] and II [R1 = H, R2 = Ph, (CH2)2Ph, C6H3-3,4-Cl2, C6H4-4-OMe; R1 = R2 = Me; R1R2 = -(CH2)5-], were prepared and assayed for their effects on H1299 lung cancer cell lines alone or with γ -radiation. Two series of quinuclidinone analogs were found to as anti-cancer agents. Of these, four interesting analogs significantly decreased cell viability in H1299 lung cancer cell lines. Two derivs. decreased cell proliferation in a dose-dependent fashion alone or in the presence of γ -radiation. Radiosensitization increased when derivative treatment preceded radiation treatment for both derivs. These preliminary studies show an evidence for both additive and synergistic cytotoxicity for treatment of lung cancer by these novel quinuclidinone analogs.

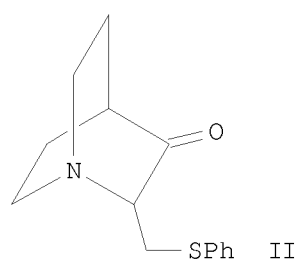
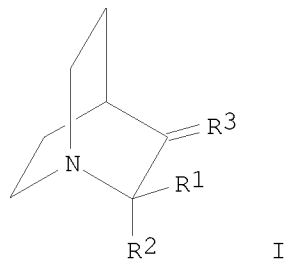
IT 865293-04-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and structure-activity studies of quinuclidinone analogs as anti-proliferative agents in lung cancer cell lines)
 RN 865293-04-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2005:1042241 CAPLUS
 DOCUMENT NUMBER: 143:326494
 TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
 INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
 PATENT ASSIGNEE(S): Aprea AB, Swed.
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010
PRIORITY APPLN. INFO.:			SE 2004-708	A 20040322
			WO 2005-SE412	W 20050322
OTHER SOURCE(S):			CASREACT 143:326494; MARPAT 143:326494	
GI				



AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R3 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μ M.

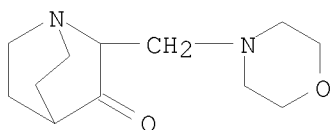
IT 41971-48-6P 343954-19-8P 586390-57-0P
 865293-03-4P 865293-04-5P 865293-05-6P
 865293-06-7P 865293-07-8P 865293-08-9P
 865293-09-0P 865293-10-3P 865293-11-4P
 865293-12-5P 865293-14-7P 865293-15-8P
 865293-16-9P 865293-17-0P 865293-18-1P
 865293-19-2P 865293-20-5P 865293-21-6P
 865293-22-7P 865293-23-8P 865293-24-9P
 865293-26-1P 865293-27-2P 865293-28-3P
 865293-29-4P 865293-30-7P 865293-31-8P
 865293-32-9P 865293-33-0P 865293-34-1P
 865293-35-2P 865293-36-3P 865293-37-4P
 865293-38-5P 865293-39-6P 865293-40-9P
 865293-41-0P 865293-42-1P 865293-43-2P
 865293-44-3P 865293-45-4P 865293-46-5P
 865293-47-6P 865293-48-7P 865293-50-1P
 865293-51-2P 865293-52-3P 865293-53-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

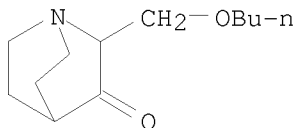
RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



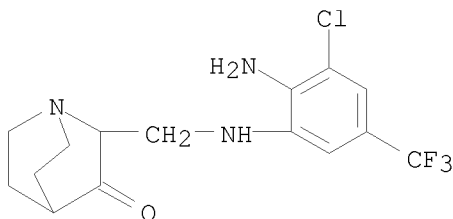
RN 343954-19-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)

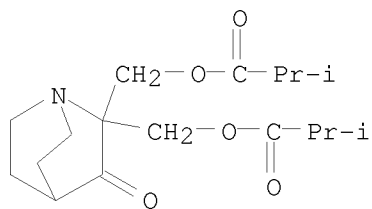


RN 586390-57-0 CAPLUS

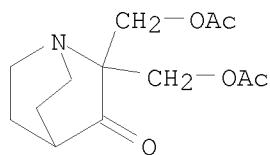
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



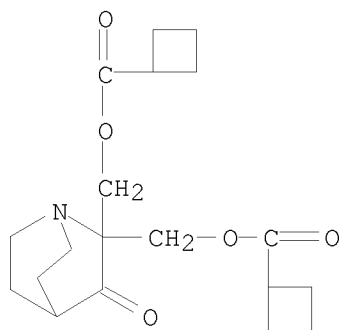
RN 865293-03-4 CAPLUS
 CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



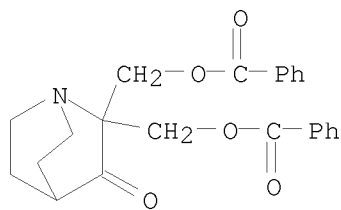
RN 865293-04-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
 CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

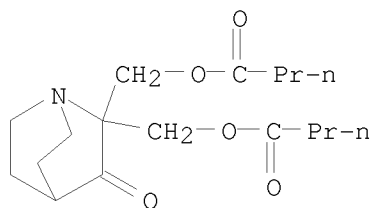


RN 865293-06-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)



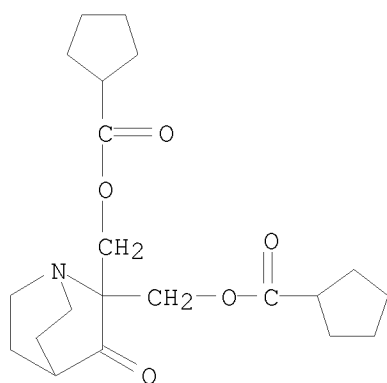
RN 865293-07-8 CAPLUS
 CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

ester (9CI) (CA INDEX NAME)



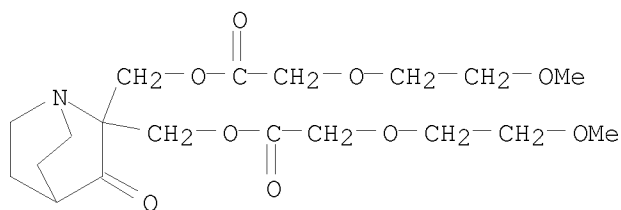
RN 865293-08-9 CAPLUS

CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



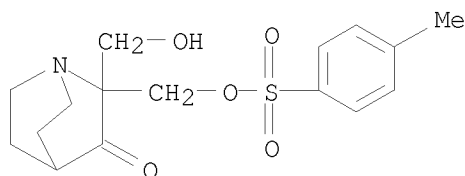
RN 865293-09-0 CAPLUS

CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



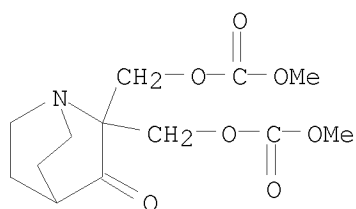
RN 865293-10-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



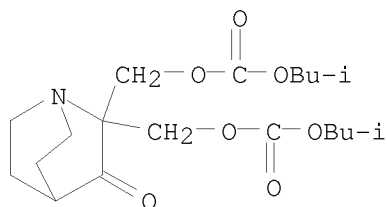
RN 865293-11-4 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



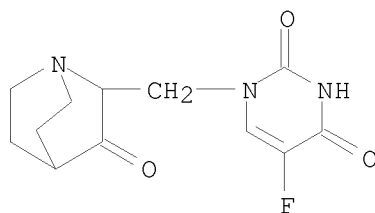
RN 865293-12-5 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



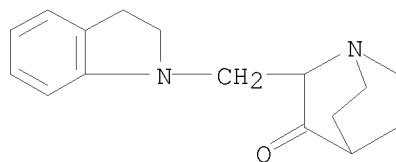
RN 865293-14-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



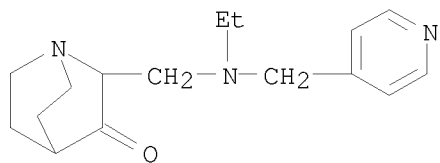
RN 865293-15-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



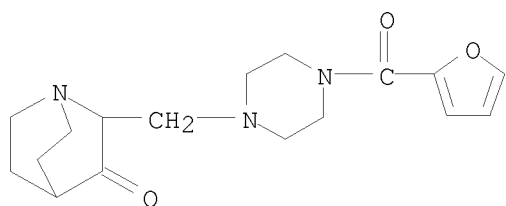
RN 865293-16-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



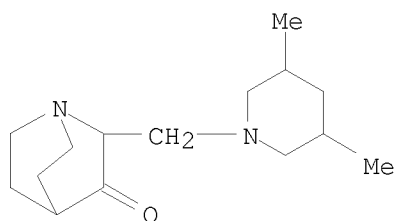
RN 865293-17-0 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



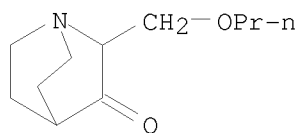
RN 865293-18-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



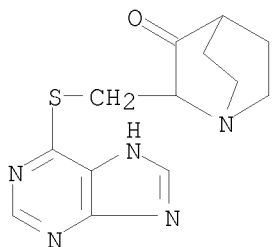
RN 865293-19-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)

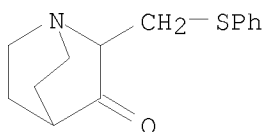


RN 865293-20-5 CAPLUS

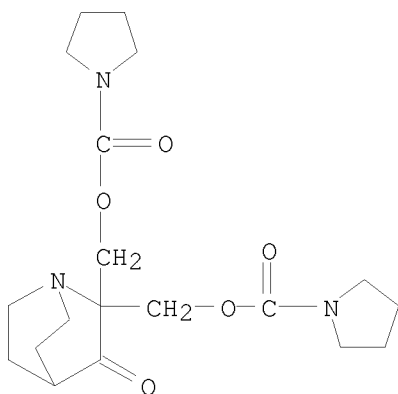
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



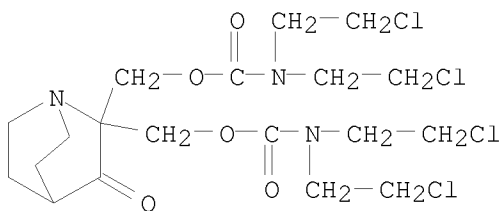
RN 865293-21-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



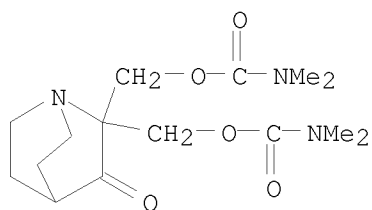
RN 865293-22-7 CAPLUS
 CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-23-8 CAPLUS
 CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

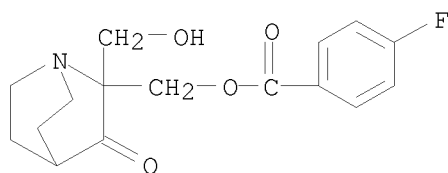


RN 865293-24-9 CAPLUS
 CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



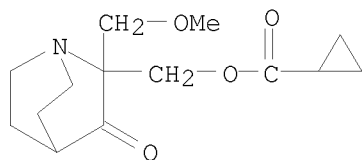
RN 865293-26-1 CAPLUS

CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



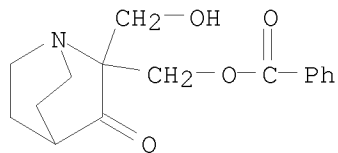
RN 865293-27-2 CAPLUS

CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



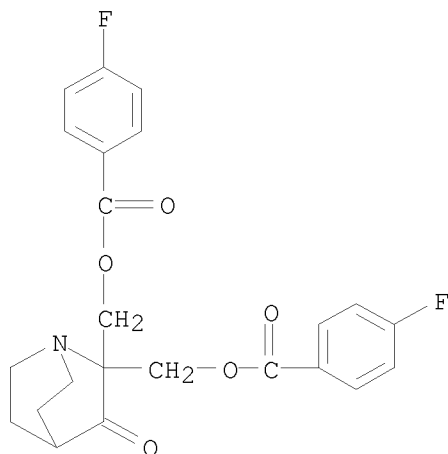
RN 865293-28-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



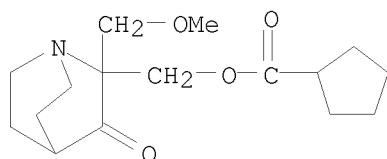
RN 865293-29-4 CAPLUS

CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-30-7 CAPLUS

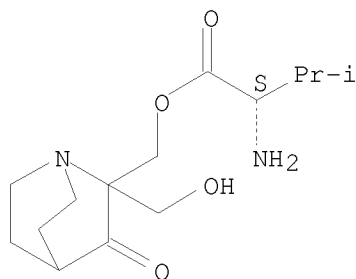
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-31-8 CAPLUS

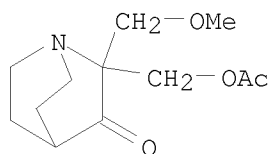
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.

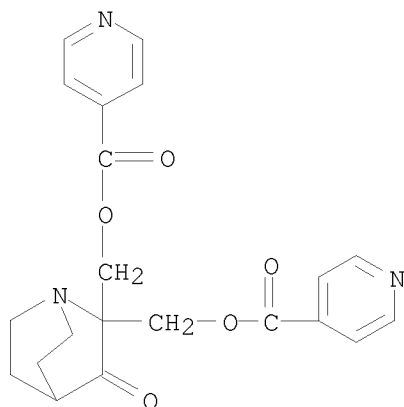


RN 865293-32-9 CAPLUS

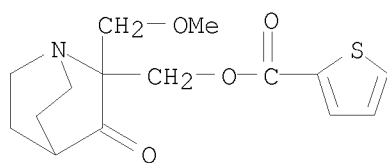
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



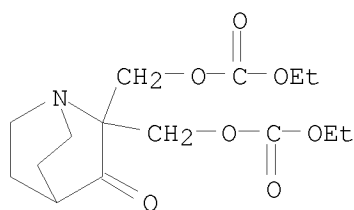
RN 865293-33-0 CAPLUS
 CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



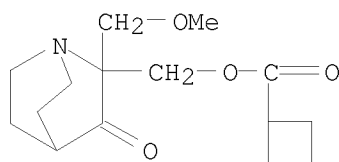
RN 865293-34-1 CAPLUS
 CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
 CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

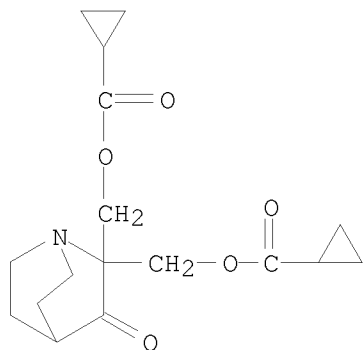


RN 865293-36-3 CAPLUS
 CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



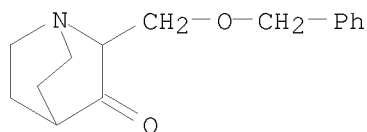
RN 865293-37-4 CAPLUS

CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



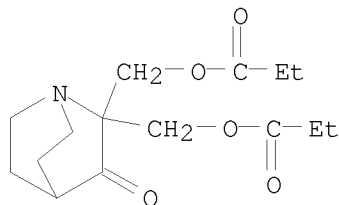
RN 865293-38-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



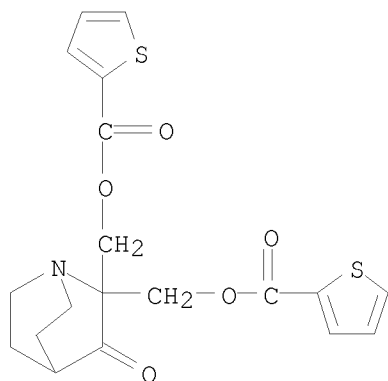
RN 865293-39-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



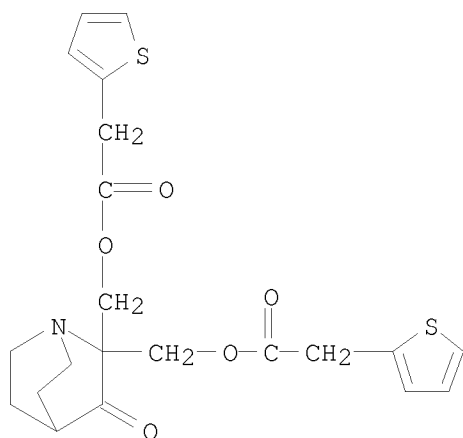
RN 865293-40-9 CAPLUS

CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



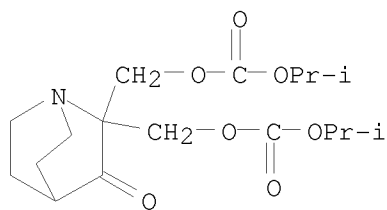
RN 865293-41-0 CAPLUS

CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



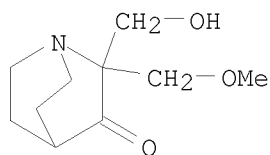
RN 865293-42-1 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

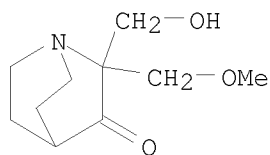
RN 865293-44-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

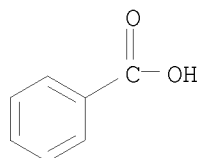
CMF C10 H17 N O3



CM 2

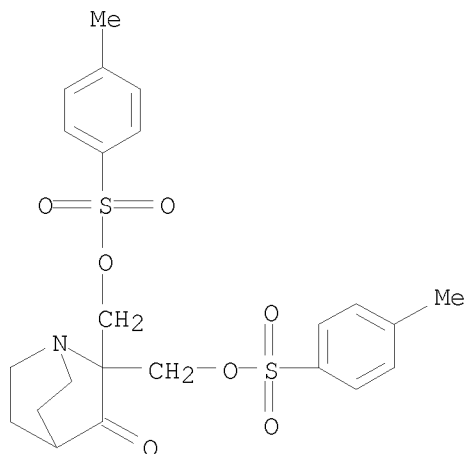
CRN 65-85-0

CMF C7 H6 O2



RN 865293-45-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



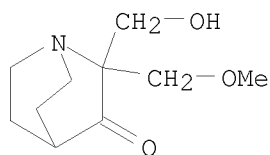
RN 865293-46-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 5291-32-7

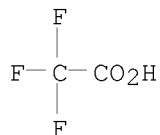
CMF C10 H17 N O3



CM 2

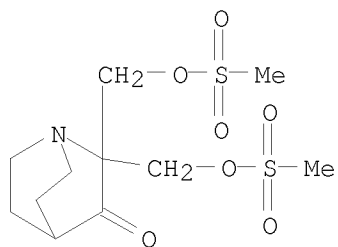
CRN 76-05-1

CMF C2 H F3 O2



RN 865293-47-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(methanesulfonyl)oxy]methyl- (CA INDEX NAME)

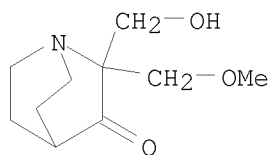


RN 865293-48-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-,
 acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

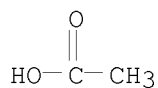
CMF C10 H17 N O3



CM 2

CRN 64-19-7

CMF C2 H4 O2

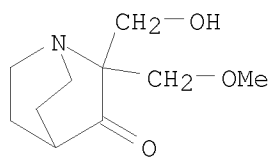


RN 865293-50-1 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-,
 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

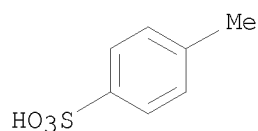
CMF C10 H17 N O3



CM 2

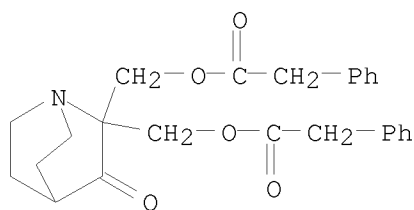
CRN 104-15-4

CMF C7 H8 O3 S



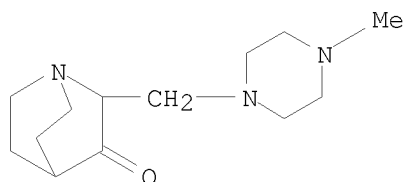
RN 865293-51-2 CAPLUS

CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



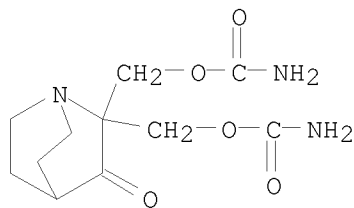
RN 865293-52-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[aminocarbonyl]oxy]methyl]- (CA INDEX NAME)



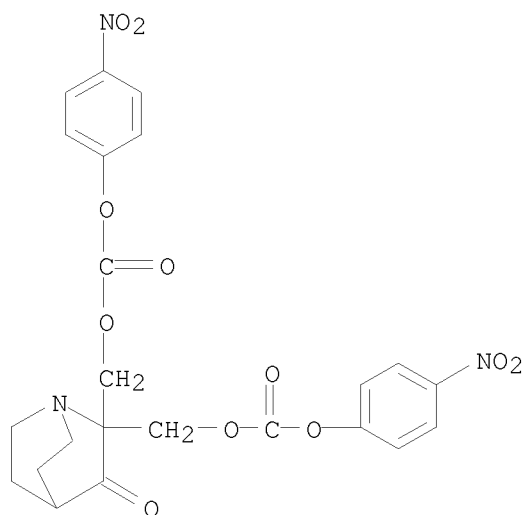
IT 865293-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

RN 865293-25-0 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

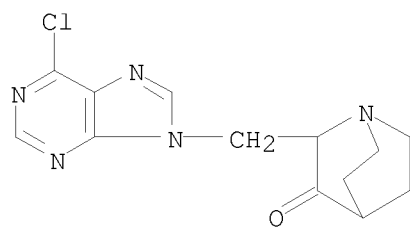
15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:240769 CAPLUS
DOCUMENT NUMBER: 136:257232
TITLE: 1-azabicyclo[2.2.2]octan-3-one derivatives and
maleimide derivatives and their use for treating
cancer tumors
INVENTOR(S): Bykov, Vladimir; Selivanova, Galina; Wiman, Klas
PATENT ASSIGNEE(S): Karolinska Innovations AB, Swed.
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002024692	A1	20020328	WO 2001-SE2008	20010919
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2423192	A1	20020328	CA 2001-2423192	20010919
AU 2001090422	A	20020402	AU 2001-90422	20010919
EP 1319000	A1	20030618	EP 2001-970421	20010919
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004509890	T	20040402	JP 2002-529102	20010919
AU 2001290422	B2	20060615	AU 2001-290422	20010919
US 20030166674	A1	20030904	US 2003-381011	20030320
US 6921765	B2	20050726		
US 20050090540	A1	20050428	US 2004-10430	20041214
US 7348330	B2	20080325		
PRIORITY APPLN. INFO.:			US 2000-234164P	P 20000920
			WO 2001-SE2008	W 20010919
			US 2003-381011	A3 20030320
OTHER SOURCE(S):	MARPAT 136:257232			
AB	1-(Propoxymethyl)maleimide, 2,2-bis(hydroxymethyl)-1-azabicyclo[2,2,2]octan-3-one, and 4 analogs selected based on structure-activity relationship studies are able to reactivate the apoptosis-inducing function of mutant p53 proteins. This reactivation is provided by restoration of sequence-specific DNA-binding activity and transcriptional transactivation function to mutant p53 proteins, and modulation of the conformation-dependent epitopes of the p53 protein. Accordingly, the substances according to the invention will be used in pharmaceutical compns. and methods for treatment of patients suffering from various types of tumors.			
IT	405096-63-1			
	RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (antitumor azabicyclooctanone derivs. and maleimide derivs. reactivate apoptosis-inducing function of mutant p53 proteins)			
RN	405096-63-1	CAPLUS		
CN	1-Azabicyclo[2.2.2]octan-3-one, 2-[(6-chloro-9H-purin-9-yl)methyl]- (CA INDEX NAME)			



REFERENCE COUNT:

23

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> s l9 and autoimmun?
      64433 AUTOIMMUN?
L11      2 L9 AND AUTOIMMUN?
```

```
=> d ibib abs hittr tot
'HITTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
```

The following are valid formats:

```
ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
      SCAN must be entered on the same line as the DISPLAY,
      e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, CLASS

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
      containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
      its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
      structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
      its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
      structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
```

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format

specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):kwic

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases

AB . . . etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of. . .

ST quinuclidinone deriv prepn cancer autoimmune heart treatment;
azabicyclooctanone prepn cancer autoimmune heart treatment

IT Antitumor agents
Autoimmune disease
Cardiovascular agents
Combination chemotherapy
Heart, disease
Human
Neoplasm
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

IT Alkaloids, preparation
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(quinuclidinone; preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

IT 148-82-3, Melphalan 15663-27-1, Cisplatin 25316-40-9, Adriamycin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
865293-09-0P 865293-10-3P 865293-11-4P
865293-12-5P 865293-13-6P 865293-14-7P
865293-15-8P 865293-16-9P 865293-17-0P
865293-18-1P 865293-19-2P 865293-20-5P
865293-21-6P 865293-22-7P 865293-23-8P
865293-24-9P 865293-26-1P 865293-27-2P
865293-28-3P 865293-29-4P 865293-30-7P
865293-31-8P 865293-32-9P 865293-33-0P
865293-34-1P 865293-35-2P 865293-36-3P
865293-37-4P 865293-38-5P 865293-39-6P
865293-40-9P 865293-41-0P 865293-42-1P
865293-43-2P 865293-44-3P 865293-45-4P
865293-46-5P 865293-47-6P 865293-48-7P
865293-50-1P 865293-51-2P 865293-52-3P
865293-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

IT 50-44-2, 6-Mercaptopurine 51-21-8, 5-Fluorouracil 71-23-8, Propanol, reactions 79-30-1, Isobutyryl chloride 98-88-4, Benzoyl chloride 100-79-8, Solketal 108-98-5, Thiophenol, reactions 141-75-3, Butyryl chloride 496-15-1, Indoline 543-27-1, Isobutyl chloroformate 1193-65-3, 3-Quinuclidinone hydrochloride 4524-93-0, Cyclopentanecarbonyl chloride 5006-22-4, Cyclobutanecarbonyl chloride 5291-26-9, 2-Methylene-3-quinuclidinone 5832-54-2 16024-55-8, 2-(2-Methoxyethoxy)acetyl chloride 33403-97-3, N-(4-Pyridylmethyl)ethylamine 35794-11-7, 3,5-Dimethylpiperidine 40172-95-0, 1-(2-Furoyl)piperazine

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer,
autoimmune and heart diseases)

IT 79-44-7P 123-75-1P, Pyrrolidine, preparation 821-48-7P,
Bis(2-chloroethyl)amine hydrochloride 5608-24-2P 7693-46-1P,
4-Nitrophenyl chloroformate 865293-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of quinuclidinone derivs. for treatment of cancer,
autoimmune and heart diseases)

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

AB . . . disorders, which are characterized by an alteration in normal neurotransmission, are also disclosed. Also disclosed are methods for treating inflammation, autoimmune disorders, pain and excess neovascularization, such as that associated with tumor growth.

IT Alzheimer's disease

Anxiety

Autoimmune disease

Central nervous system, disease

Hyperkinesia

Inflammation

Neoplasm

Pain

Parkinson's disease

Schizophrenia

Sepsis

(medicaments; preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

IT 273748-51-9P

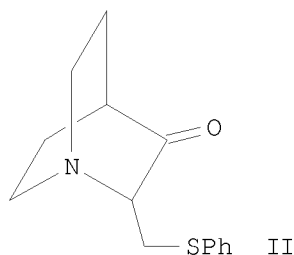
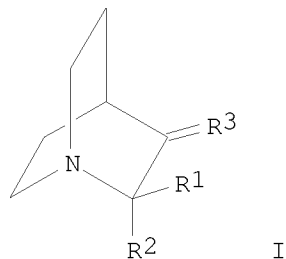
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of; preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

=> d ibib abs hitstr l11 tot

ACCESSION NUMBER: 2005:1042241 CAPLUS
 DOCUMENT NUMBER: 143:326494
 TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
 INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
 PATENT ASSIGNEE(S): Aprea AB, Swed.
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010
PRIORITY APPLN. INFO.:			SE 2004-708	A 20040322
			WO 2005-SE412	W 20050322
OTHER SOURCE(S):			CASREACT 143:326494; MARPAT 143:326494	
GI				



AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R3 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μ M.

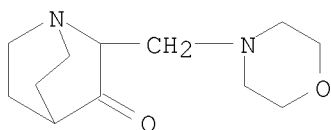
IT 41971-48-6P 343954-19-8P 586390-57-0P
 865293-03-4P 865293-04-5P 865293-05-6P
 865293-06-7P 865293-07-8P 865293-08-9P
 865293-09-0P 865293-10-3P 865293-11-4P
 865293-12-5P 865293-14-7P 865293-15-8P
 865293-16-9P 865293-17-0P 865293-18-1P
 865293-19-2P 865293-20-5P 865293-21-6P
 865293-22-7P 865293-23-8P 865293-24-9P
 865293-26-1P 865293-27-2P 865293-28-3P
 865293-29-4P 865293-30-7P 865293-31-8P
 865293-32-9P 865293-33-0P 865293-34-1P
 865293-35-2P 865293-36-3P 865293-37-4P
 865293-38-5P 865293-39-6P 865293-40-9P
 865293-41-0P 865293-42-1P 865293-43-2P
 865293-44-3P 865293-45-4P 865293-46-5P
 865293-47-6P 865293-48-7P 865293-50-1P
 865293-51-2P 865293-52-3P 865293-53-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

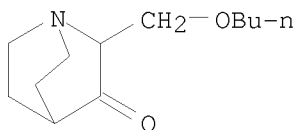
RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



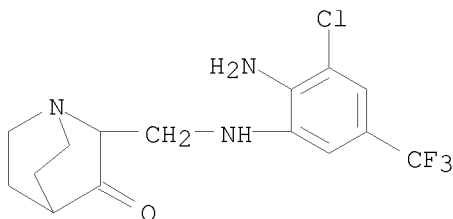
RN 343954-19-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)

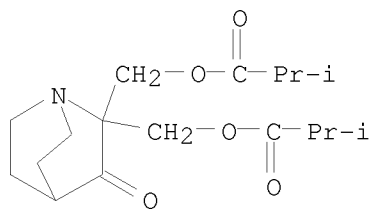


RN 586390-57-0 CAPLUS

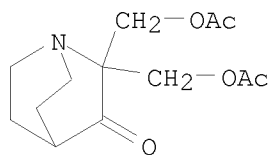
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



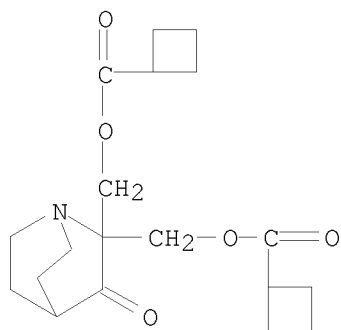
RN 865293-03-4 CAPLUS
 CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



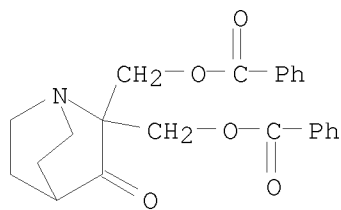
RN 865293-04-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
 CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

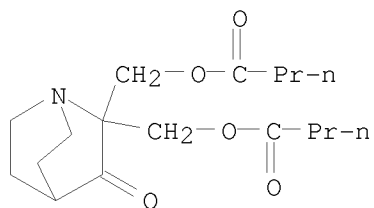


RN 865293-06-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)



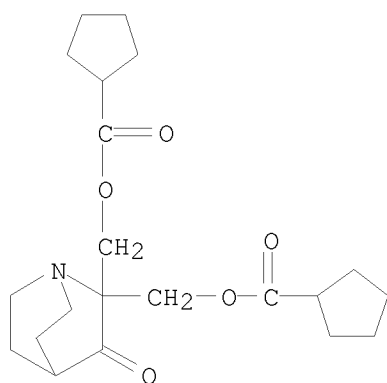
RN 865293-07-8 CAPLUS
 CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

ester (9CI) (CA INDEX NAME)



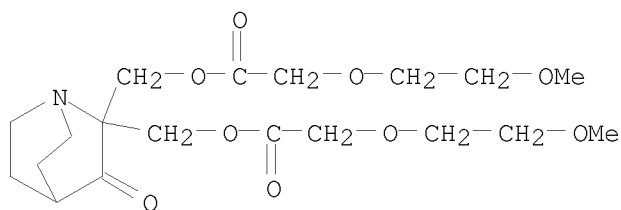
RN 865293-08-9 CAPLUS

CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



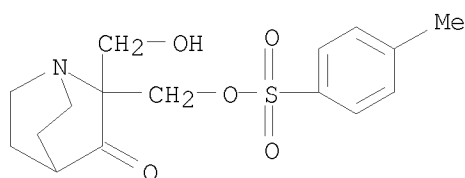
RN 865293-09-0 CAPLUS

CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



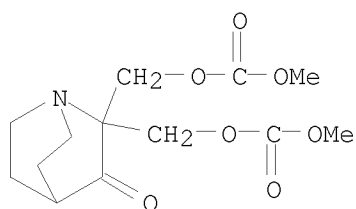
RN 865293-10-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



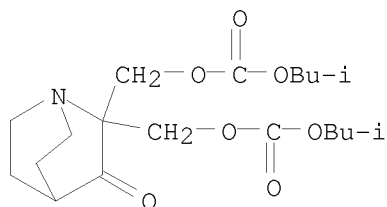
RN 865293-11-4 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



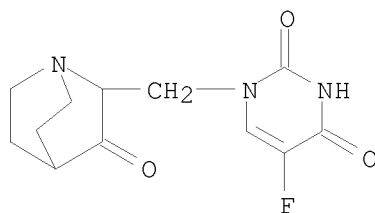
RN 865293-12-5 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



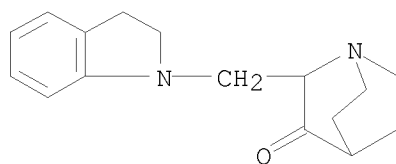
RN 865293-14-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



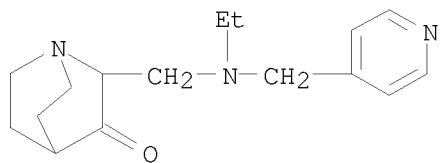
RN 865293-15-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



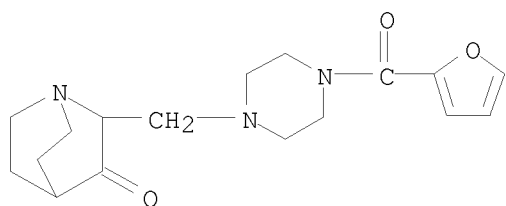
RN 865293-16-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



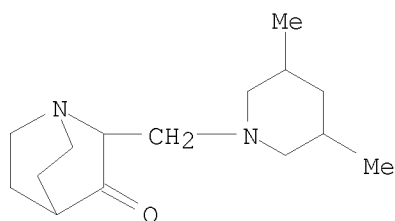
RN 865293-17-0 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



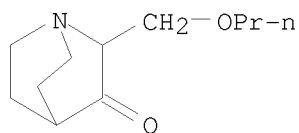
RN 865293-18-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



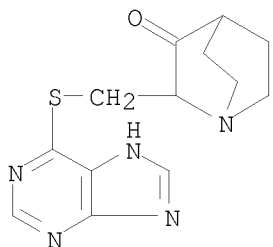
RN 865293-19-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)

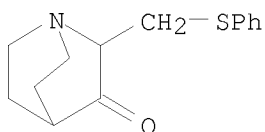


RN 865293-20-5 CAPLUS

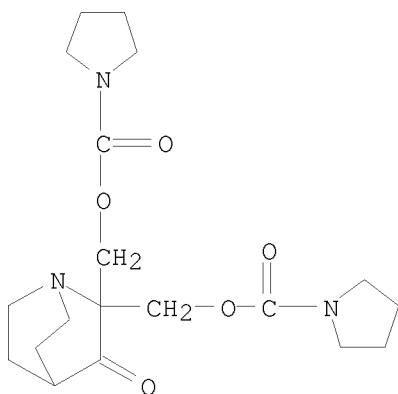
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



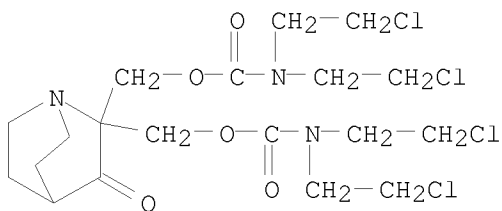
RN 865293-21-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



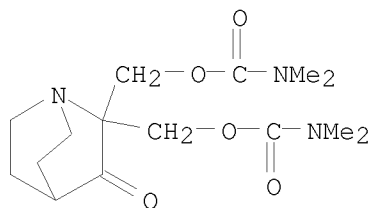
RN 865293-22-7 CAPLUS
 CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-23-8 CAPLUS
 CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

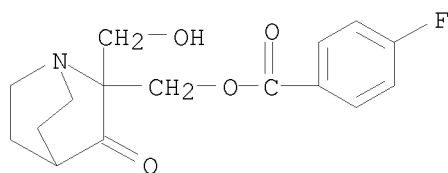


RN 865293-24-9 CAPLUS
 CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



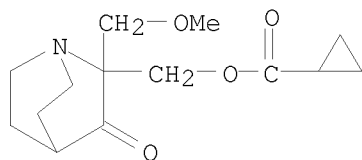
RN 865293-26-1 CAPLUS

CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



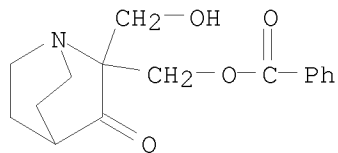
RN 865293-27-2 CAPLUS

CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



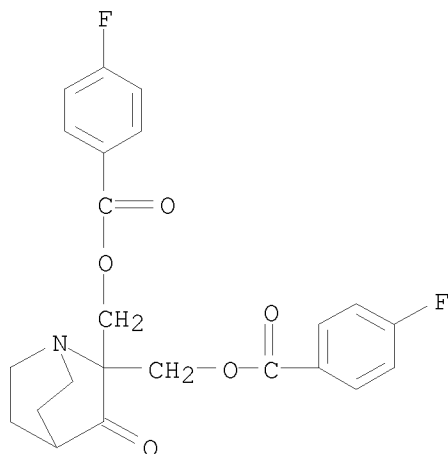
RN 865293-28-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



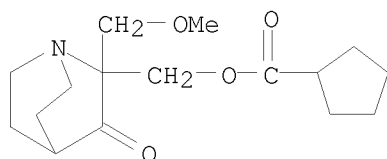
RN 865293-29-4 CAPLUS

CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-30-7 CAPLUS

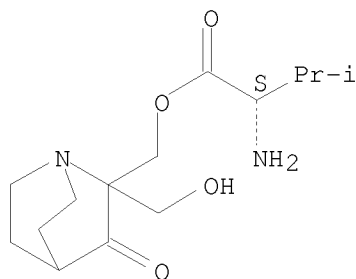
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-31-8 CAPLUS

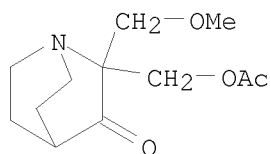
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.



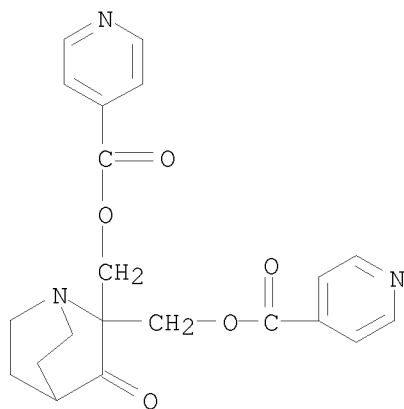
RN 865293-32-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



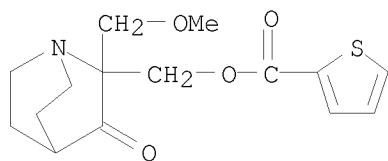
RN 865293-33-0 CAPLUS

CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



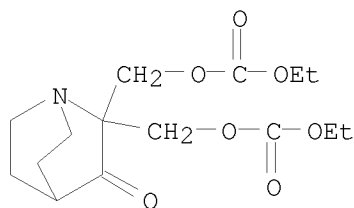
RN 865293-34-1 CAPLUS

CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



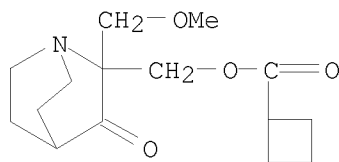
RN 865293-35-2 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)



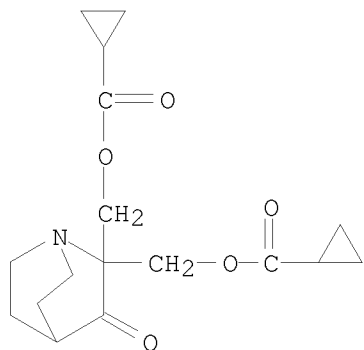
RN 865293-36-3 CAPLUS

CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



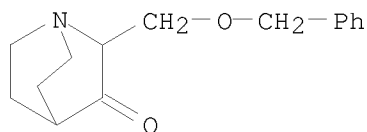
RN 865293-37-4 CAPLUS

CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



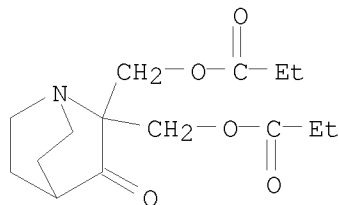
RN 865293-38-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



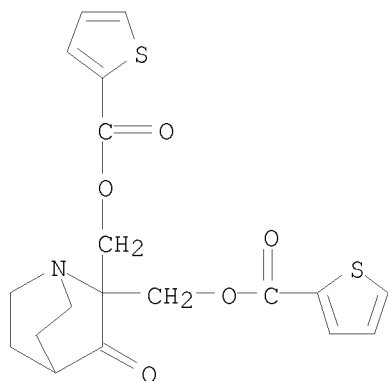
RN 865293-39-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



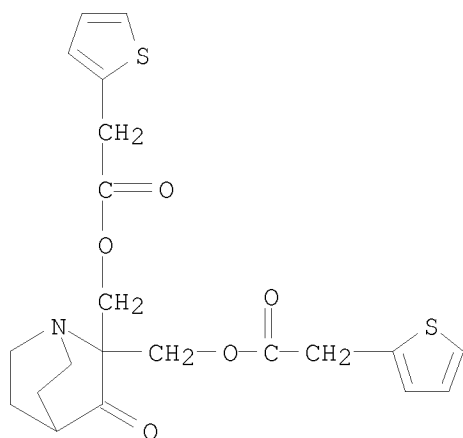
RN 865293-40-9 CAPLUS

CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



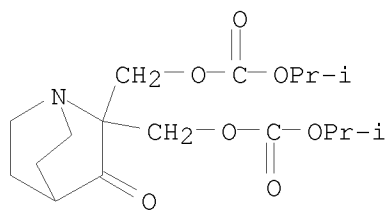
RN 865293-41-0 CAPLUS

CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



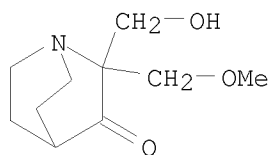
RN 865293-42-1 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

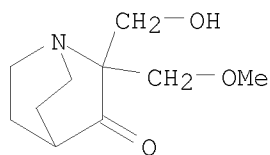
RN 865293-44-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

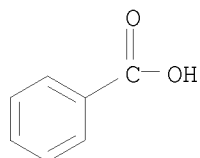
CMF C10 H17 N O3



CM 2

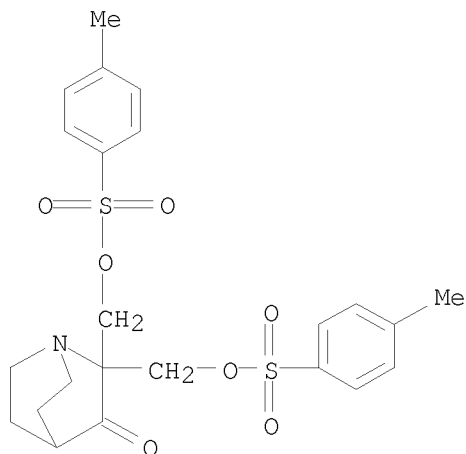
CRN 65-85-0

CMF C7 H6 O2



RN 865293-45-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



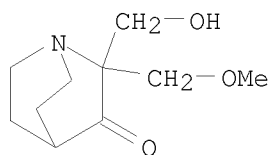
RN 865293-46-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 5291-32-7

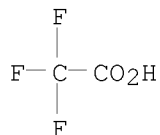
CMF C10 H17 N O3



CM 2

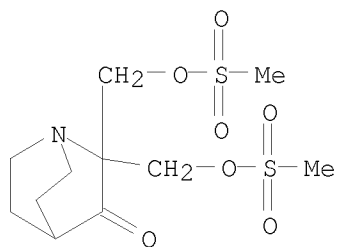
CRN 76-05-1

CMF C2 H F3 O2



RN 865293-47-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)



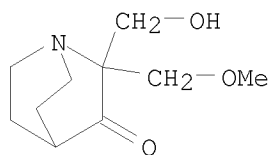
RN 865293-48-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

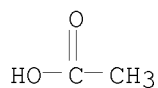
CMF C10 H17 N O3



CM 2

CRN 64-19-7

CMF C2 H4 O2



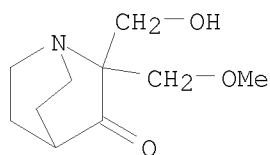
RN 865293-50-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

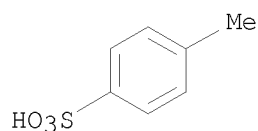
CMF C10 H17 N O3



CM 2

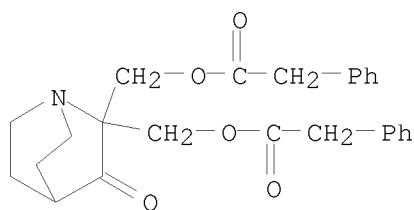
CRN 104-15-4

CMF C7 H8 O3 S



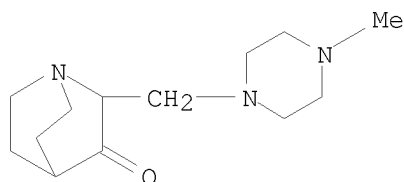
RN 865293-51-2 CAPLUS

CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



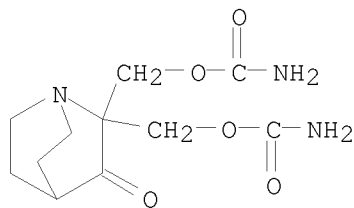
RN 865293-52-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[aminocarbonyl]oxy]methyl]- (CA INDEX NAME)



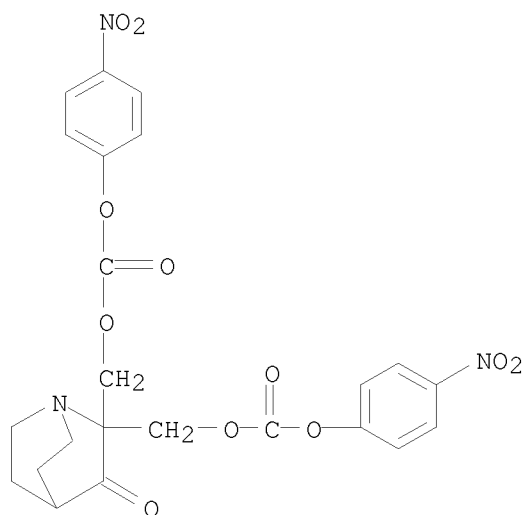
IT 865293-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

RN 865293-25-0 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

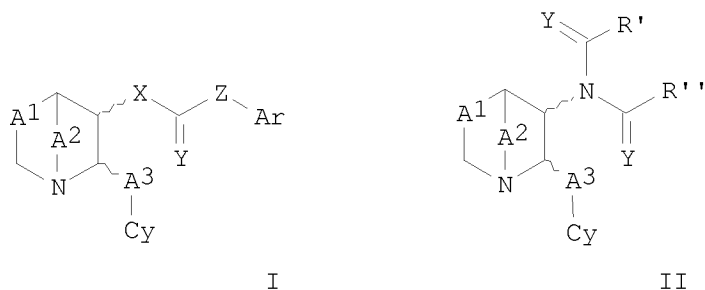
15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:3665 CAPLUS
DOCUMENT NUMBER: 140:77298
TITLE: Preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes and methods of treatment using these compounds
INVENTOR(S): Mazurov, Anatoly A.; Klucik, Jozef; Miao, Lan; Seamans, Angela S.; Phillips, Teresa Youngpeter; Schmitt, Jeffrey Daniel; Miller, Craig Harrison
PATENT ASSIGNEE(S): Targacept, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 162,129.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	-----	-----	-----
US 20040002513	A1	20040101	US 2003-372642	20030221
US 6953855	B2	20051011		
US 6432975	B1	20020813	US 1998-210113	19981211
US 20030045523	A1	20030306	US 2002-162129	20020604
AU 2004215386	A1	20040910	AU 2004-215386	20040220
CA 2514135	A1	20040910	CA 2004-2514135	20040220
WO 2004076449	A2	20040910	WO 2004-US5044	20040220
WO 2004076449	A3	20041216		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1594869	A2	20051116	EP 2004-713356	20040220
EP 1594869	B1	20071219		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2004007708	A	20060214	BR 2004-7708	20040220
CN 1751041	A	20060322	CN 2004-80004736	20040220
JP 2006518746	T	20060817	JP 2006-503737	20040220
AT 381563	T	20080115	AT 2004-713356	20040220
NZ 541794	A	20080328	NZ 2004-541794	20040220
US 20050255040	A1	20051117	US 2005-157119	20050620
ZA 2005006515	A	20060628	ZA 2005-6515	20050815
MX 2005PA08926	A	20051005	MX 2005-PA8926	20050822
IN 2005KN01718	A	20070323	IN 2005-KN1718	20050829
NO 2005004052	A	20051021	NO 2005-4052	20050831
US 20060247270	A1	20061102	US 2006-458231	20060718
PRIORITY APPLN. INFO.:			US 1998-210113	A1 19981211
			US 2002-162129	A2 20020604
			US 2003-372642	A 20030221
			WO 2004-US5044	A 20040220
			US 2005-157119	A1 20050620
OTHER SOURCE(S):	MARPAT 140:77298			
GI				

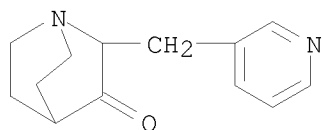


AB The present invention relates to 3-substituted-2-(arylalkyl)-1-azabicycloalkanes I [A1 = (CH₂)_n; A2 = (CH₂)_m; A3 = (CH₂)_p; m, n = 1, 2; p = 1 - 4; X = O, NR'; Z = NR', covalent bond, A; A = CR'R'', CR'R''CR'R'', CR':CR', C.tplbond.C (wherein, when Z = bond or A, X = N); Ar = (un)substituted carbocyclic, heterocyclic monocyclic or fused polycyclic aryl; Cy = (un)substituted 5- or 6-membered heteroarom. ring; wavy lines = relative or absolute stereochem. (cis or trans, R or S); R', R'' = H, (un)branched C1-8-alkyl, C3-8-cycloalkyl, heterocyclyl, aryl, arylalkyl {wherein, substituents = alkyl, alkenyl, heterocyclyl, cycloalkyl, (un)substituted aryl, (un)substituted arylalkyl, F, Cl, Br, I, OR', NR'R'', CF₃, CN, NO₂, C.tplbond.CR', SR', N₃, C(:O)NR'R'', NR'C(:O)R'', C(:O)R', C(:O)OR', OC(:O)R', O(CR'R'')rC(:O)R', O(CR'R'')rNR''C(:O)R', O(CR'R'')rNR''SO₂R', OC(:O)NR'R'', NR'C(:O)OR'', SO₂R', SO₂NR'R'', NR'SO₂R''}; R'R'' = ring; r = 1 - 6] and II, methods of preparing the compds. and methods of treatment using the compds. The azabicycloalkanes generally are azabicycloheptanes, azabicyclooctanes, or azabicyclononanes. The aryl group in the arylalkyl moiety is a 5- or 6-membered ring heteroarom., preferably 3-pyridinyl and 5-pyrimidinyl moieties, and the alkyl group is typically a C 1-4 alkyl. The substituent at the 3-position of the 1-azabicycloalkane is a carbonyl group-containing moiety, such as an amide, carbamate, urea, thioamide, thiocarbamate, thiourea or similar functionality. The compds. exhibit activity at nicotinic acetylcholine receptors (nAChRs), particularly the α7 nAChR subtype, and are useful towards modulating neurotransmission and the release of ligands involved in neurotransmission. Methods for preventing or treating conditions and disorders, including central nervous system (CNS) disorders, which are characterized by an alteration in normal neurotransmission, are also disclosed. Also disclosed are methods for treating inflammation, autoimmune disorders, pain and excess neovascularization, such as that associated with tumor growth.

IT 273748-51-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of; preparation of 3-substituted-2(arylalkyl)-1-
azabicycloalkanes exhibiting activity at nicotinic acetylcholine
receptors)

RN 273748-51-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(3-pyridinylmethyl)- (CA INDEX NAME)



REFERENCE COUNT:

59

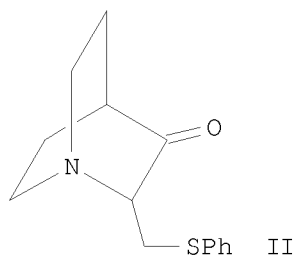
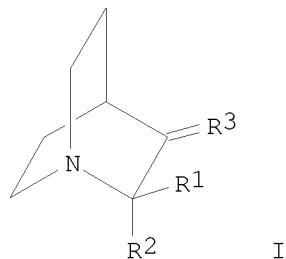
THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


```
=> s l9 and heart
      363973 HEART
      30453 HEARTS
      366123 HEART
              (HEART OR HEARTS)
L12      2 L9 AND HEART

=> d ibib abs hitstr tot
```

ACCESSION NUMBER: 2005:1042241 CAPLUS
 DOCUMENT NUMBER: 143:326494
 TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
 INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
 PATENT ASSIGNEE(S): Aprea AB, Swed.
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010
PRIORITY APPLN. INFO.:			SE 2004-708	A 20040322
			WO 2005-SE412	W 20050322
OTHER SOURCE(S):			CASREACT 143:326494; MARPAT 143:326494	
GI				



AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μ M.

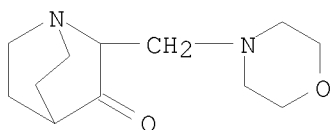
IT 41971-48-6P 343954-19-8P 586390-57-0P
 865293-03-4P 865293-04-5P 865293-05-6P
 865293-06-7P 865293-07-8P 865293-08-9P
 865293-09-0P 865293-10-3P 865293-11-4P
 865293-12-5P 865293-14-7P 865293-15-8P
 865293-16-9P 865293-17-0P 865293-18-1P
 865293-19-2P 865293-20-5P 865293-21-6P
 865293-22-7P 865293-23-8P 865293-24-9P
 865293-26-1P 865293-27-2P 865293-28-3P
 865293-29-4P 865293-30-7P 865293-31-8P
 865293-32-9P 865293-33-0P 865293-34-1P
 865293-35-2P 865293-36-3P 865293-37-4P
 865293-38-5P 865293-39-6P 865293-40-9P
 865293-41-0P 865293-42-1P 865293-43-2P
 865293-44-3P 865293-45-4P 865293-46-5P
 865293-47-6P 865293-48-7P 865293-50-1P
 865293-51-2P 865293-52-3P 865293-53-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

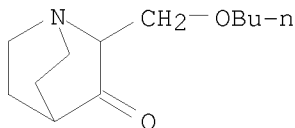
RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



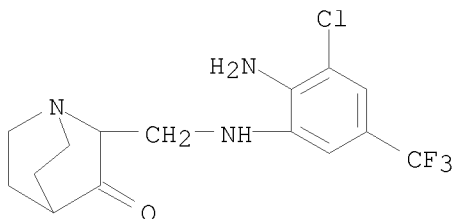
RN 343954-19-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)

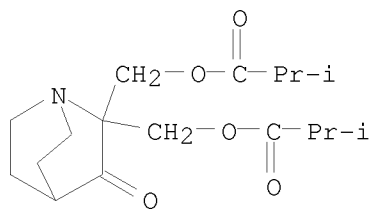


RN 586390-57-0 CAPLUS

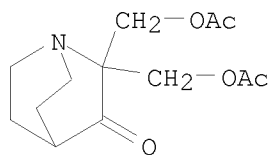
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



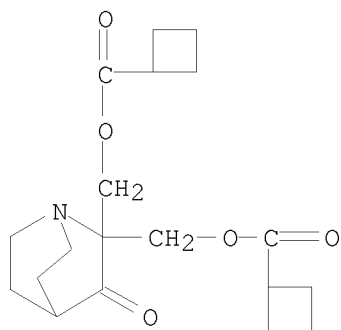
RN 865293-03-4 CAPLUS
 CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



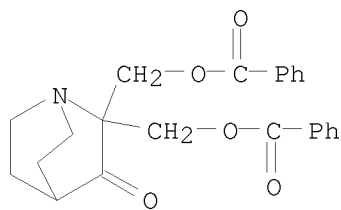
RN 865293-04-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
 CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

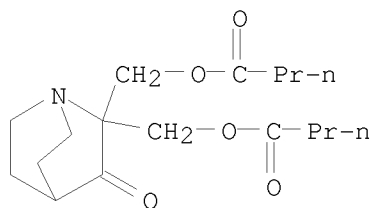


RN 865293-06-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)



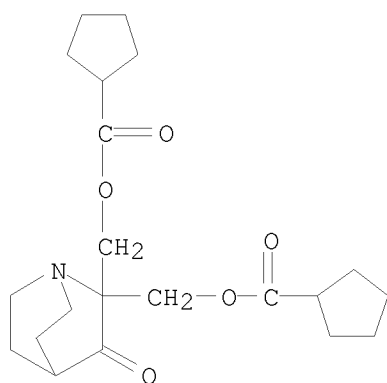
RN 865293-07-8 CAPLUS
 CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

ester (9CI) (CA INDEX NAME)



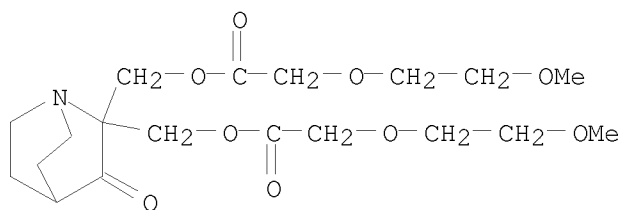
RN 865293-08-9 CAPLUS

CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



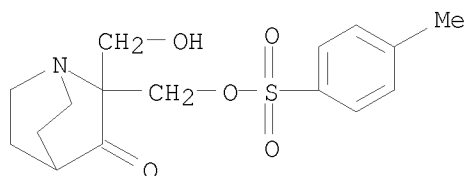
RN 865293-09-0 CAPLUS

CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



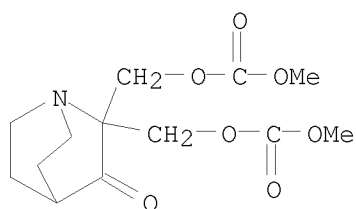
RN 865293-10-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



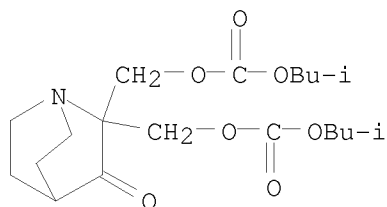
RN 865293-11-4 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



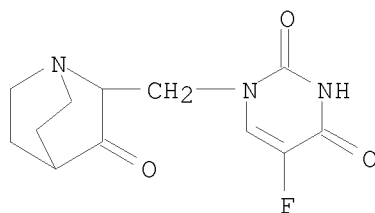
RN 865293-12-5 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



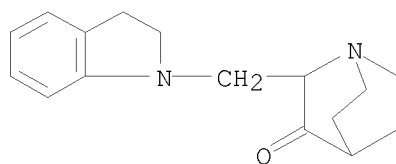
RN 865293-14-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



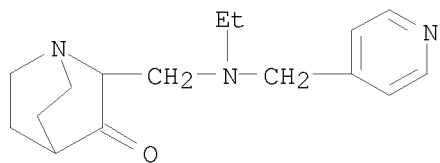
RN 865293-15-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



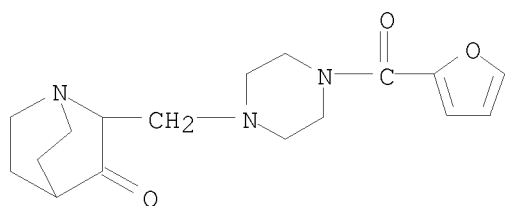
RN 865293-16-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



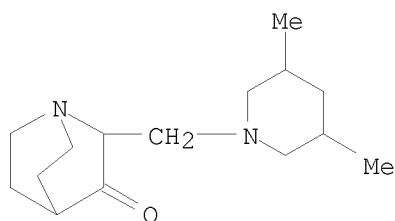
RN 865293-17-0 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



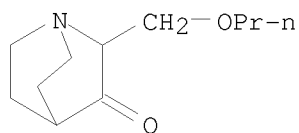
RN 865293-18-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



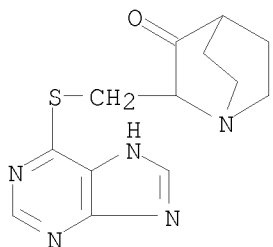
RN 865293-19-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)

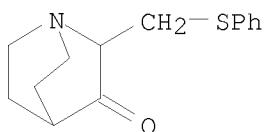


RN 865293-20-5 CAPLUS

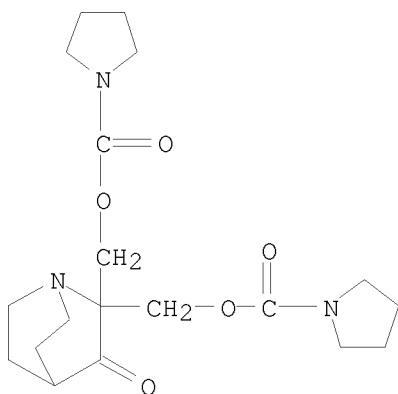
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



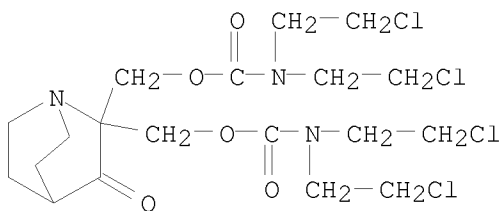
RN 865293-21-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



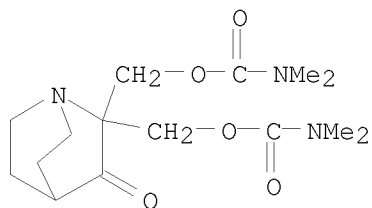
RN 865293-22-7 CAPLUS
 CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-23-8 CAPLUS
 CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

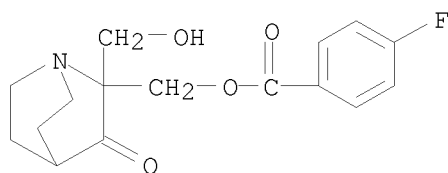


RN 865293-24-9 CAPLUS
 CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



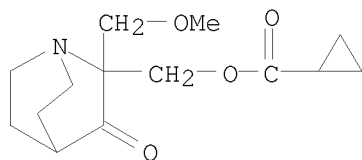
RN 865293-26-1 CAPLUS

CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



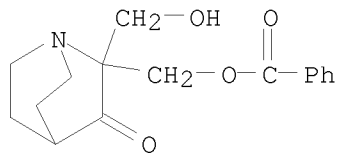
RN 865293-27-2 CAPLUS

CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



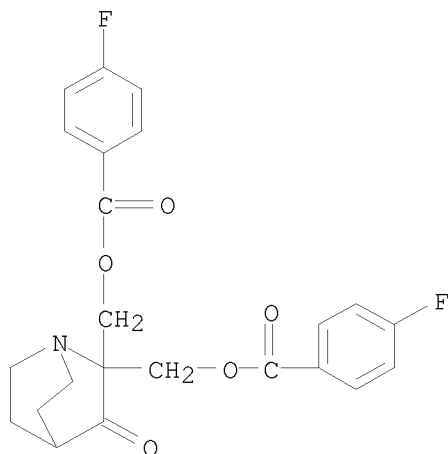
RN 865293-28-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



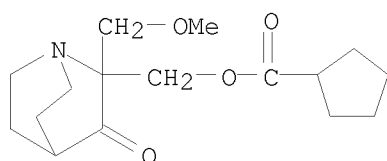
RN 865293-29-4 CAPLUS

CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-30-7 CAPLUS

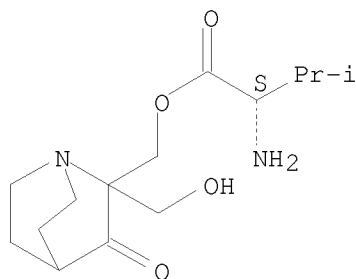
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-31-8 CAPLUS

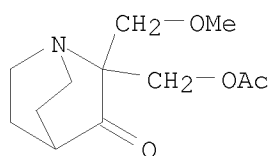
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.



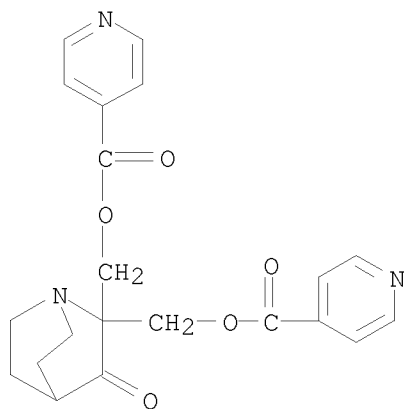
RN 865293-32-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



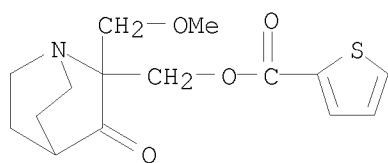
RN 865293-33-0 CAPLUS

CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



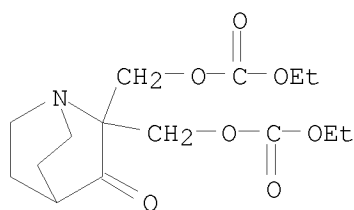
RN 865293-34-1 CAPLUS

CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



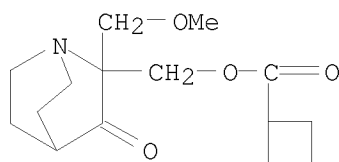
RN 865293-35-2 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)



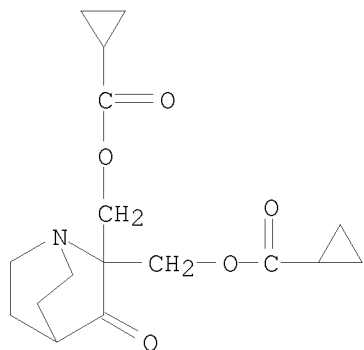
RN 865293-36-3 CAPLUS

CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



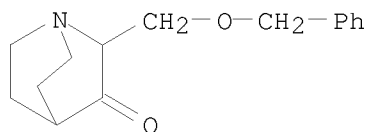
RN 865293-37-4 CAPLUS

CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



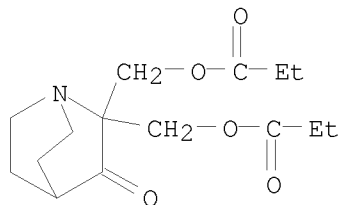
RN 865293-38-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



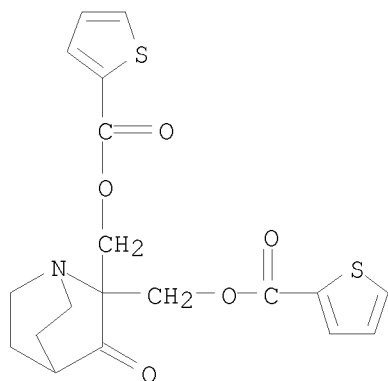
RN 865293-39-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



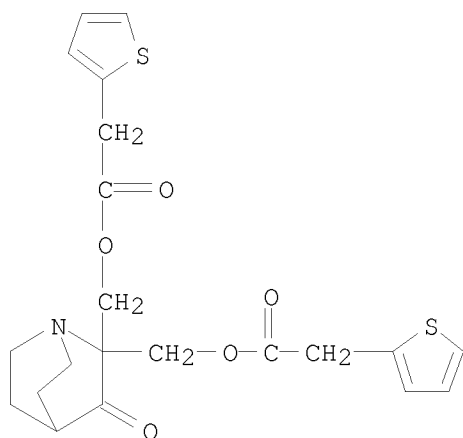
RN 865293-40-9 CAPLUS

CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



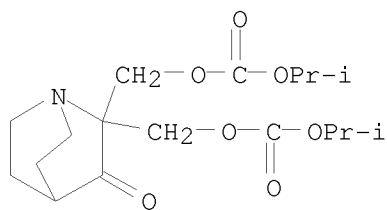
RN 865293-41-0 CAPLUS

CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



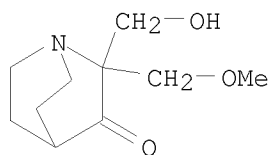
RN 865293-42-1 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

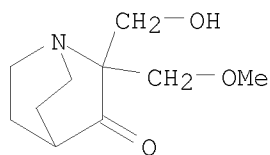
RN 865293-44-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

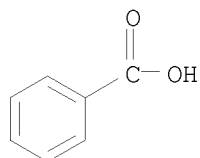
CMF C10 H17 N O3



CM 2

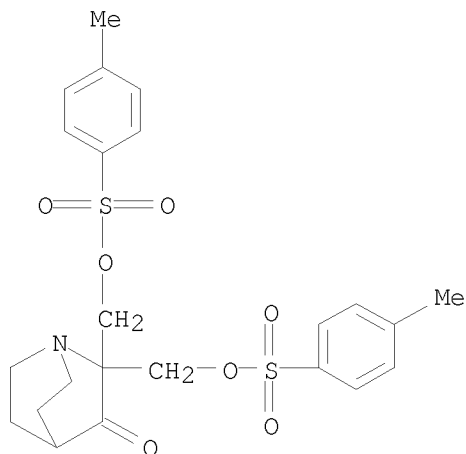
CRN 65-85-0

CMF C7 H6 O2



RN 865293-45-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



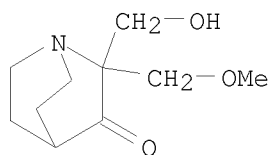
RN 865293-46-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 5291-32-7

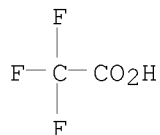
CMF C10 H17 N O3



CM 2

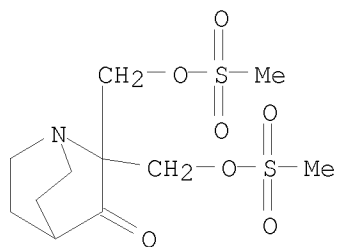
CRN 76-05-1

CMF C2 H F3 O2



RN 865293-47-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)

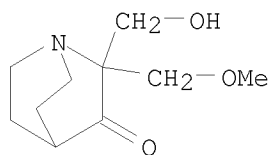


RN 865293-48-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-,
 acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

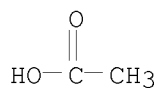
CMF C10 H17 N O3



CM 2

CRN 64-19-7

CMF C2 H4 O2

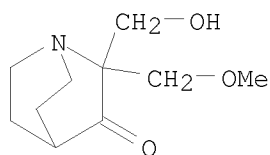


RN 865293-50-1 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-,
 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

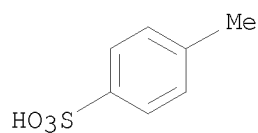
CMF C10 H17 N O3



CM 2

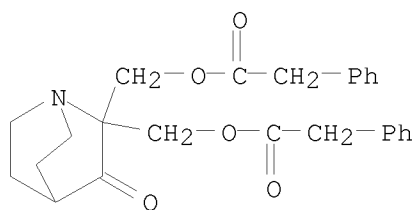
CRN 104-15-4

CMF C7 H8 O3 S



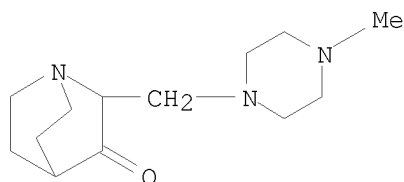
RN 865293-51-2 CAPLUS

CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



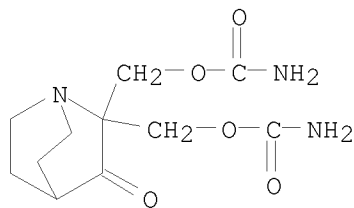
RN 865293-52-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[aminocarbonyl]oxy]methyl]- (CA INDEX NAME)



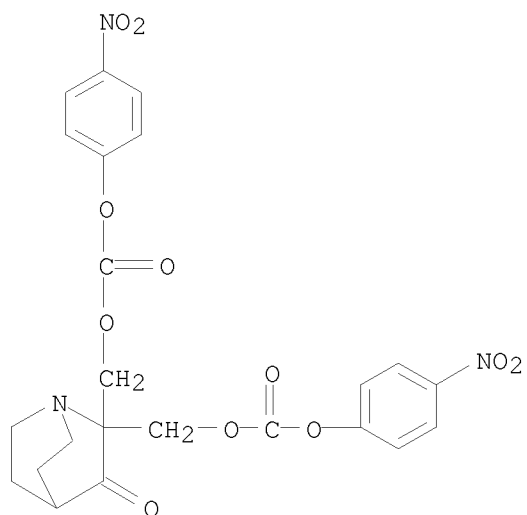
IT 865293-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

RN 865293-25-0 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

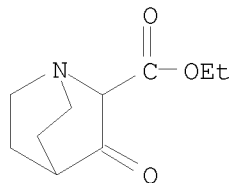
ACCESSION NUMBER: 1991:199680 CAPLUS
 DOCUMENT NUMBER: 114:199680
 ORIGINAL REFERENCE NO.: 114:33481a,33484a
 TITLE: Preparation of renin-inhibitory di-, tri-, and tetrapeptide cardiovascular drug
 INVENTOR(S): Greenlee, William J.; Broeke, Jan Ten
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: Eur. Pat. Appl., 35 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 389127	A1	19900926	EP 1990-302145	19900228
R: CH, DE, FR, GB, IT, LI, NL				
US 5049548	A	19910917	US 1989-319448	19890303
CA 2011327	A1	19900903	CA 1990-2011327	19900302
JP 02300200	A	19901212	JP 1990-51593	19900302
PRIORITY APPLN. INFO.:			US 1989-319448	A 19890303
OTHER SOURCE(S):			CASREACT 114:199680; MARPAT 114:199680	

AB The peptides ABEGTJ [A = (un)substituted heterocyclyl; B = NA1CH[(CH2)mR]CO; E = absent or NA1CH[(CH2)nR1]CO; A1, R = H, alkyl; R1 = H, aryl, etc.; m = 0, 1, 2; n = 1-4; G = HNC[(CH2)mR2]CH(OH)CHR3CO, HNC[(CH2)mR2]CH(OH)CO, etc.; R2 = alkyl, aryl, (un)substituted cycloalkyl; R3 = H, alkyl, alkenyl, etc.; T = absent or NHCH[(CH2)m]RCO; J = Y(CH2)x(CHR3)y(CH2)zR4; Y = O, NH, etc.; R4 = H, OH, alkyl; x, y = 0, 1; z = 0, 1-4] are prepared as renin inhibitors, useful as drugs for the treatment of hypertension and congestive heart failure (no data). To a solution of 0.09 g 3-quinuclidinone and 4.15 g Phe-O-tert-Bu in 50 mL MeOH was added a solution of 2.95 g Na cyanoborohydride in 13 mL MeOH and 5.78 g pyridine-HCl, to give N α -(quinuclidine-3(RS)-yl)phenylalanine tert-Bu ester-HCl.

IT 52763-22-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reductive coupling of, to protected amino acids)

RN 52763-22-1 CAPLUS
 CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



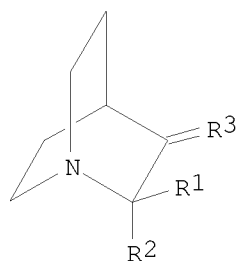
● HCl

```
=> s l9 and hyperproliferative
      1982 HYPERPROLIFERATIVE
L13      1 L9 AND HYPERPROLIFERATIVE

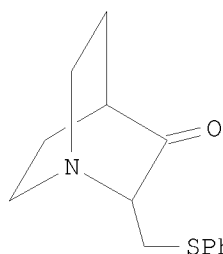
=> d ibib abs hitstr tot
```

ACCESSION NUMBER: 2005:1042241 CAPLUS
 DOCUMENT NUMBER: 143:326494
 TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
 INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
 PATENT ASSIGNEE(S): Aprea AB, Swed.
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010
PRIORITY APPLN. INFO.:			SE 2004-708	A 20040322
			WO 2005-SE412	W 20050322
OTHER SOURCE(S):			CASREACT 143:326494; MARPAT 143:326494	
GI				



I



II

AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative diseases, e.g. cancer as well as autoimmune

diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μ M.

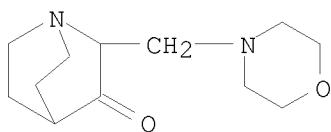
IT 41971-48-6P 343954-19-8P 586390-57-0P
 865293-03-4P 865293-04-5P 865293-05-6P
 865293-06-7P 865293-07-8P 865293-08-9P
 865293-09-0P 865293-10-3P 865293-11-4P
 865293-12-5P 865293-14-7P 865293-15-8P
 865293-16-9P 865293-17-0P 865293-18-1P
 865293-19-2P 865293-20-5P 865293-21-6P
 865293-22-7P 865293-23-8P 865293-24-9P
 865293-26-1P 865293-27-2P 865293-28-3P
 865293-29-4P 865293-30-7P 865293-31-8P
 865293-32-9P 865293-33-0P 865293-34-1P
 865293-35-2P 865293-36-3P 865293-37-4P
 865293-38-5P 865293-39-6P 865293-40-9P
 865293-41-0P 865293-42-1P 865293-43-2P
 865293-44-3P 865293-45-4P 865293-46-5P
 865293-47-6P 865293-48-7P 865293-50-1P
 865293-51-2P 865293-52-3P 865293-53-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

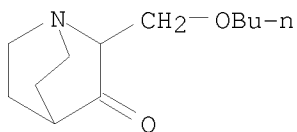
RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



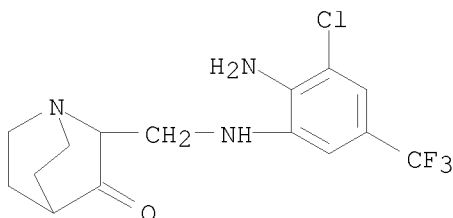
RN 343954-19-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)

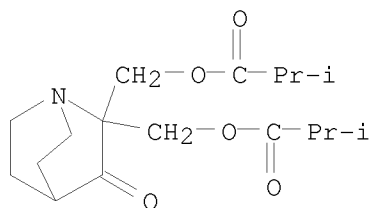


RN 586390-57-0 CAPLUS

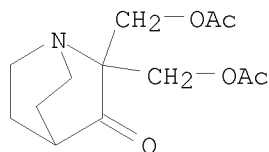
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



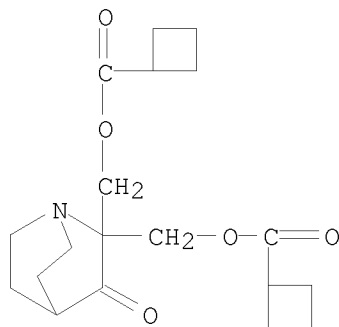
RN 865293-03-4 CAPLUS
 CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



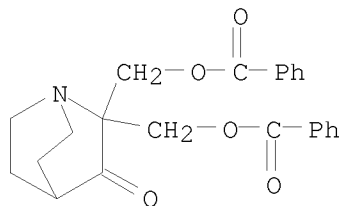
RN 865293-04-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



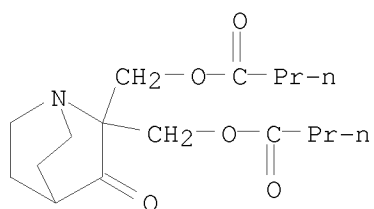
RN 865293-05-6 CAPLUS
 CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-06-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)

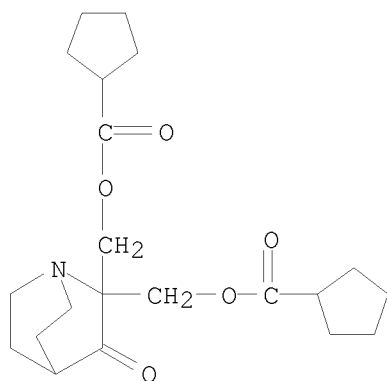


RN 865293-07-8 CAPLUS
 CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



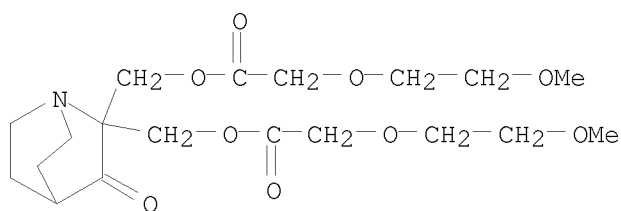
RN 865293-08-9 CAPLUS

CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



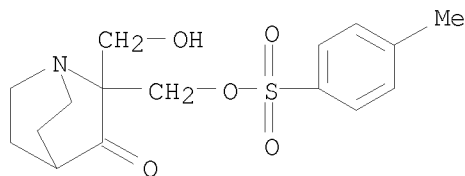
RN 865293-09-0 CAPLUS

CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



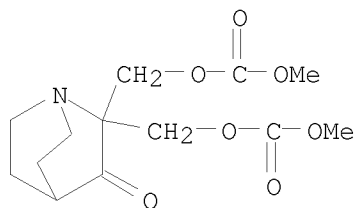
RN 865293-10-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



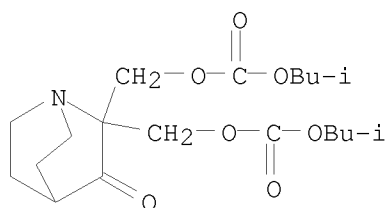
RN 865293-11-4 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



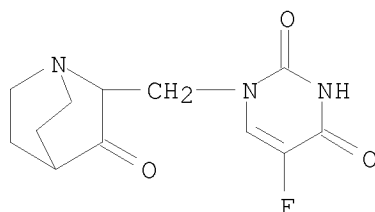
RN 865293-12-5 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



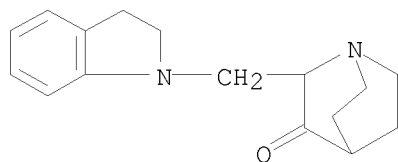
RN 865293-14-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



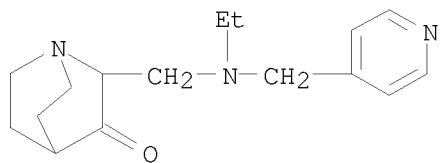
RN 865293-15-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



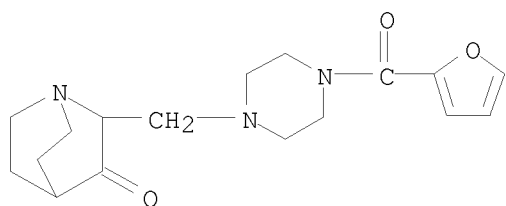
RN 865293-16-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



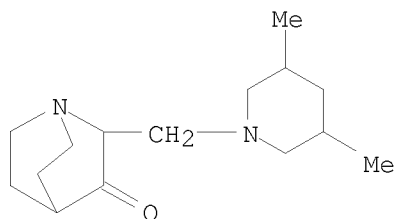
RN 865293-17-0 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



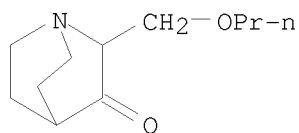
RN 865293-18-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



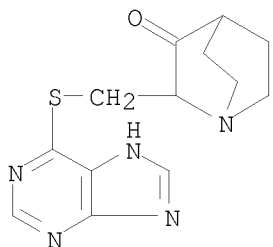
RN 865293-19-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)

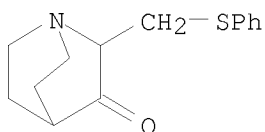


RN 865293-20-5 CAPLUS

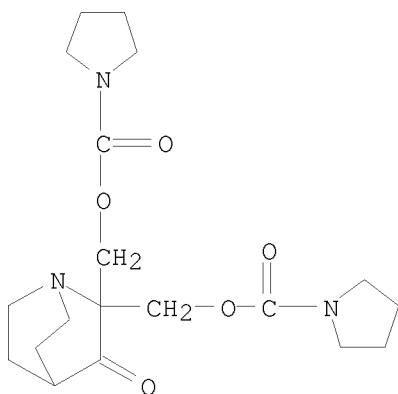
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



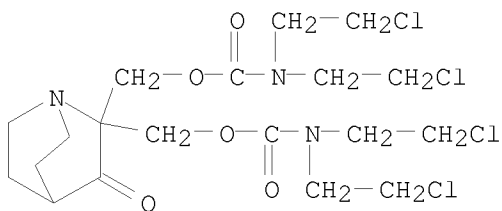
RN 865293-21-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



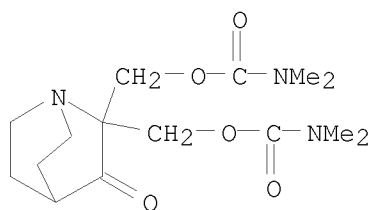
RN 865293-22-7 CAPLUS
 CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-23-8 CAPLUS
 CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

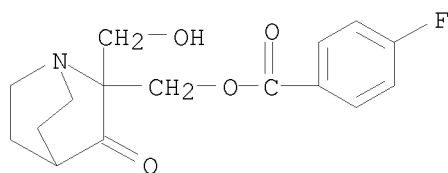


RN 865293-24-9 CAPLUS
 CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



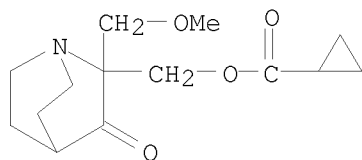
RN 865293-26-1 CAPLUS

CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



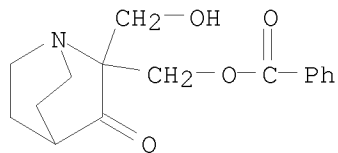
RN 865293-27-2 CAPLUS

CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



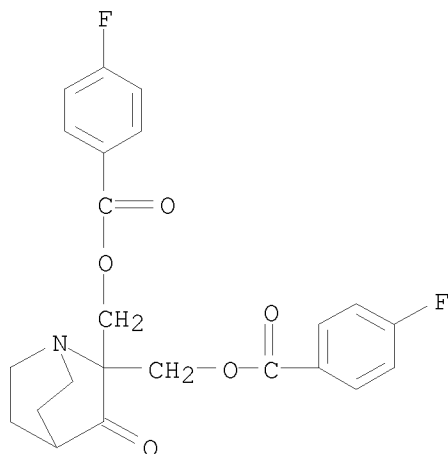
RN 865293-28-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



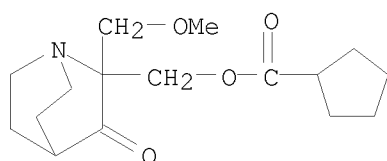
RN 865293-29-4 CAPLUS

CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-30-7 CAPLUS

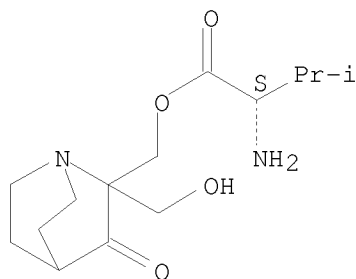
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-31-8 CAPLUS

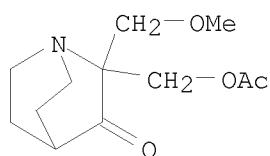
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.

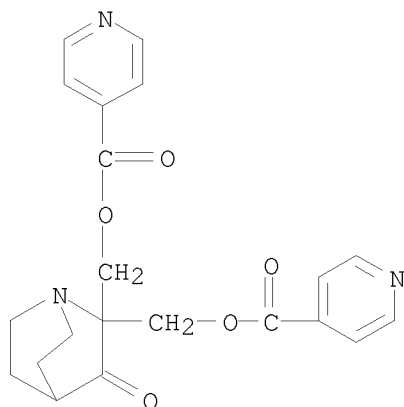


RN 865293-32-9 CAPLUS

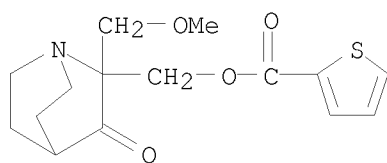
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



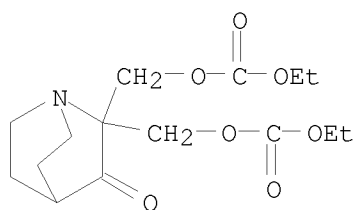
RN 865293-33-0 CAPLUS
 CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



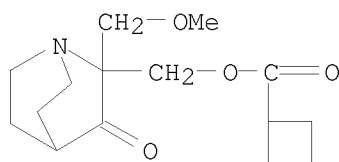
RN 865293-34-1 CAPLUS
 CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
 CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

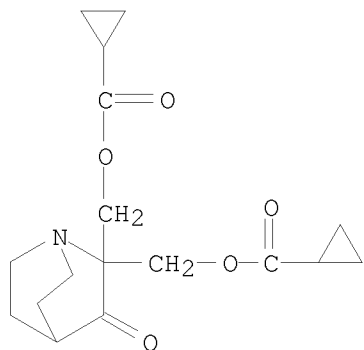


RN 865293-36-3 CAPLUS
 CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



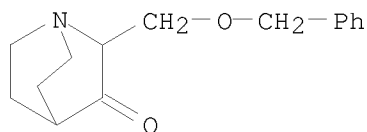
RN 865293-37-4 CAPLUS

CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



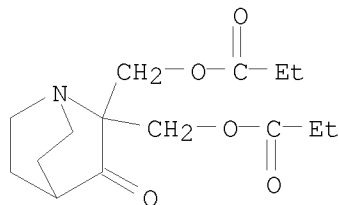
RN 865293-38-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



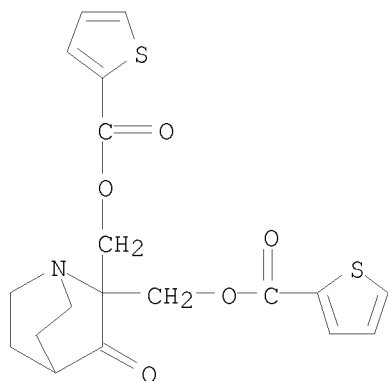
RN 865293-39-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



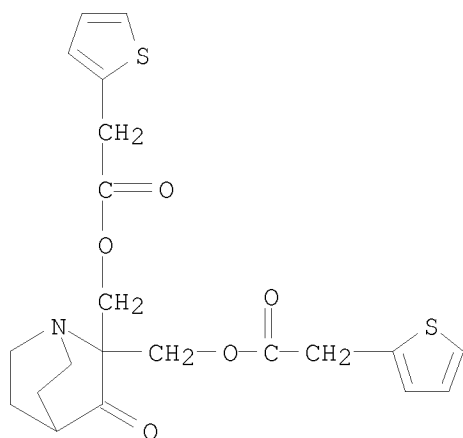
RN 865293-40-9 CAPLUS

CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



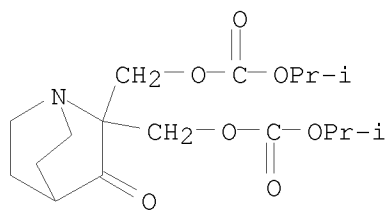
RN 865293-41-0 CAPLUS

CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



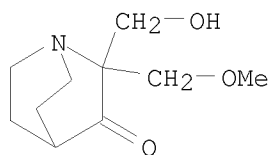
RN 865293-42-1 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

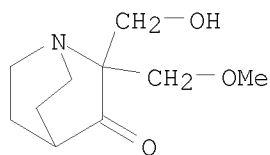


● HCl

RN 865293-44-3 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-,
 benzoate (1:1) (CA INDEX NAME)

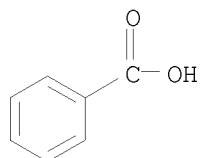
CM 1

CRN 5291-32-7
 CMF C10 H17 N O3

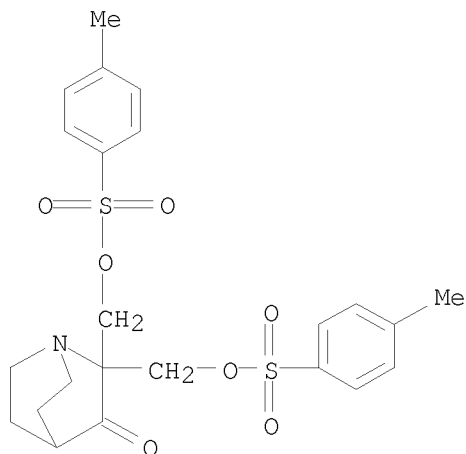


CM 2

CRN 65-85-0
 CMF C7 H6 O2



RN 865293-45-4 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]met
 hyl]- (CA INDEX NAME)



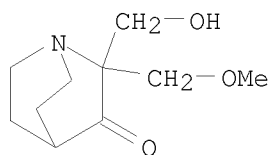
RN 865293-46-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 5291-32-7

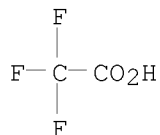
CMF C10 H17 N O3



CM 2

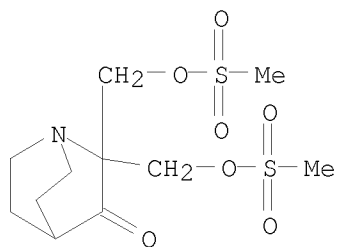
CRN 76-05-1

CMF C2 H F3 O2



RN 865293-47-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(methylsulfonyl)oxy]methyl- (CA INDEX NAME)



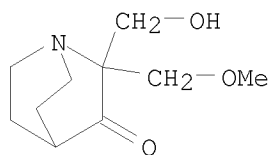
RN 865293-48-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

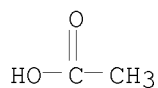
CMF C10 H17 N O3



CM 2

CRN 64-19-7

CMF C2 H4 O2



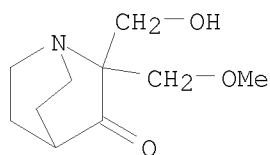
RN 865293-50-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7

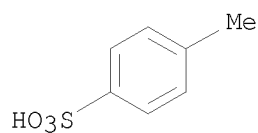
CMF C10 H17 N O3



CM 2

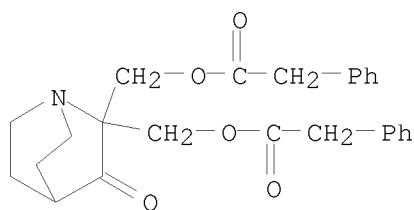
CRN 104-15-4

CMF C7 H8 O3 S



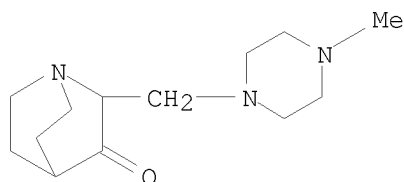
RN 865293-51-2 CAPLUS

CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



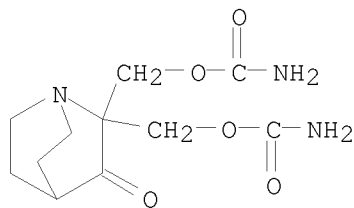
RN 865293-52-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[aminocarbonyl]oxy]methyl]- (CA INDEX NAME)



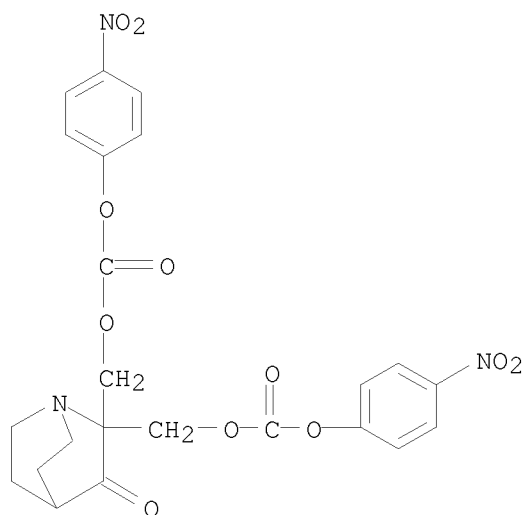
IT 865293-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

RN 865293-25-0 CAPLUS

CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


```
=> s 19 and diseases?  
      1202101 DISEAS?  
L14      25 L9 AND DISEAS?  
  
=> s 19 and py<2003  
      22930206 PY<2003  
L15      134 L9 AND PY<2003  
  
=> d ibib abs hitstr 100-134
```

ACCESSION NUMBER: 1974:413478 CAPLUS
 DOCUMENT NUMBER: 81:13478
 ORIGINAL REFERENCE NO.: 81:2171a,2174a
 TITLE: Benzopyrans
 INVENTOR(S): Wright, Howard Bernard; Horrom, Bruce W.
 PATENT ASSIGNEE(S): Abbott Laboratories
 SOURCE: Ger. Offen., 23 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2351734	A1	19740418	DE 1973-2351734	19731015 <--
US 3915996	A	19751028	US 1973-367027	19730608 <--
CA 992080	A1	19760629	CA 1973-180946	19730913 <--
ZA 7307326	A	19740828	ZA 1973-7326	19730914 <--
GB 1438833	A	19760609	GB 1973-44478	19730921 <--
AU 7360663	A	19750327	AU 1973-60663	19730925 <--
FI 59597	B	19810529	FI 1973-3019	19730927 <--
FI 59597	C	19810910		
NL 7313595	A	19740418	NL 1973-13595	19731003 <--
JP 49072259	A	19740712	JP 1973-112902	19731009 <--
FR 2202887	A1	19740510	FR 1973-36784	19731015 <--
NO 141089	B	19791001	NO 1973-4000	19731015 <--
NO 141089	C	19800109		
DK 143029	B	19810316	DK 1973-5575	19731015 <--
DK 143029	C	19811026		
BE 806152	A1	19740416	BE 1973-136757	19731016 <--
CH 591468	A5	19770915	CH 1973-14626	19731016 <--
FI 8100118	A	19810116	FI 1981-118	19810116 <--
PRIORITY APPLN. INFO.:			US 1972-298132	A 19721016
			US 1973-367027	A 19730608
			FI 1973-3019	A 19730927

GI For diagram(s), see printed CA Issue.

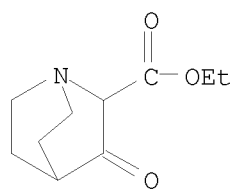
AB Four benzopyrans [I and II, X = CH₂, CH₂CH₂, or N(CH₂C.tplbond.CH)-CH₂; R = Me] and (or) their salts with HCl or HBr, useful as analgesics, were prepared by reaction of resorcinols with β -oxo-esters, e.g. III (R₁ = CH₂Ph) (IV) in MeSO₃H to give corresponding I or II (RR = O), followed by reaction with MeMgBr, and optionally hydrogenolytic cleavage of the N-protecting CH₂-Ph group. Thus, 3,5-(HO)2C₆H₃CHMe(CH₂)3C₆H₄F-4 reacted with IV.HCl in MeSO₃H in the presence of POCl₃ to give I.HCl [X = N(CH₂Ph)CH₂, RR = O] (V.HCl). V reacted with Me-MgBr in PhOMe to give, after treatment with dilute H₂SO₄, I [X = N(CH₂Ph)CH₂, R = Me], which on hydrogenolysis and reaction with HC.tplbond.CCH₂Br gave I [X = N(CH₂C.tplbond.CH)CH₂, R = Me].

IT 52763-22-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with resorcinols)

RN 52763-22-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester,
 hydrochloride (9CI) (CA INDEX NAME)



● HCl

L15 ANSWER 101 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:77753 CAPLUS

DOCUMENT NUMBER: 80:77753

ORIGINAL REFERENCE NO.: 80:12485a,12488a

TITLE: Transition metal chemistry of quinuclidinone-containing ligands. II. Spectral and magnetic properties of some transition metal complexes containing 2-(N-morpholinylmethyl)-3-quinuclidinone and related ligands

AUTHOR(S): Dickinson, Richard C.; Long, Gary J.

CORPORATE SOURCE: Dep. Chem., Univ. Missouri, Rolla, MO, USA

SOURCE: Inorganic Chemistry (1974), 13(2), 262-9

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complexes of Co(II), Ni(II), and Fe(II) halides with 2-(N-morpholinyl)methyl-3-quinuclidinone (L) were prepared by adding the appropriate metal salt to the ligand in alc. solns. The complexes have pseudotetrahedral microsymmetry around the central metal ion as indicated by their spectral and magnetic properties; the coordination sphere contains 1 bidentate N-bonded ligand and 2 halide atoms. Ligand field band assignments, metal-halide stretching frequencies, and magnetic susceptibility data are given for each of the complexes. The Co(II) and Ni(II) perchlorate complexes of L were also prepared, and each contains 2 bidentate ligands which provide a tetrahedral ligand field that is stronger than for the halide complexes. The apparent preference of the ligand for 1-to-1 metal-to-ligand coordination and the consequent tetrahedral structures result from a combination of the size of the quinuclidine group and the rigidity of the 5-membered chelate ring formed by the coordinated ligand. In addition to these pseudotetrahedral complexes, an octahedral Ni chloride complex which contains bridging chloride ligands is reported. A cobaltous thiocyanate complex also has an octahedral structure in the solid state and a tetrahedral structure in solution

IT 41971-48-6P 42886-08-8P 42892-78-4P

42892-79-5P 42892-80-8P 42892-81-9P

42892-82-0P 42892-83-1P 42892-84-2P

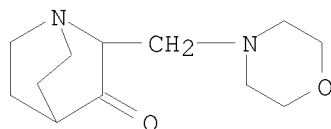
42892-85-3P 42892-86-4P 42892-87-5P

42942-73-4P 43021-09-6P 54218-39-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



RN 42886-08-8 CAPLUS

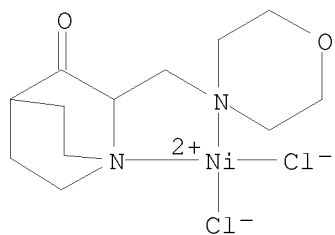
CN Nickel, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 48175-79-7

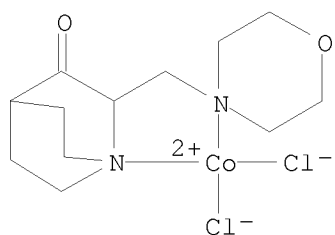
CMF C12 H20 Cl2 N2 Ni O2

CCI CCS



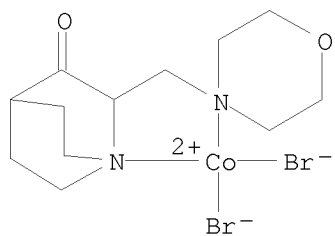
RN 42892-78-4 CAPLUS

CN Cobalt, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



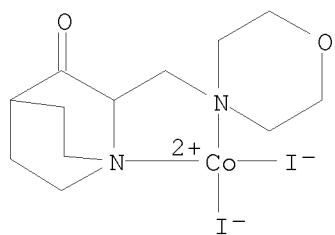
RN 42892-79-5 CAPLUS

CN Cobalt, dibromo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



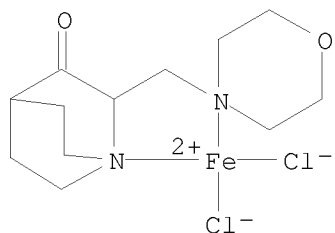
RN 42892-80-8 CAPLUS

CN Cobalt, diiodo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)

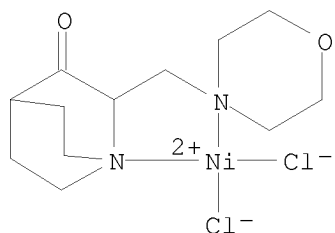


RN 42892-81-9 CAPLUS

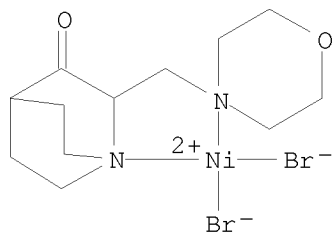
CN Iron, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



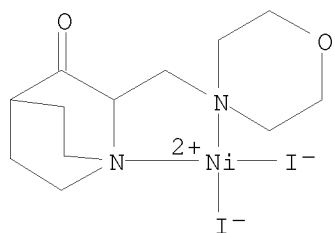
RN 42892-82-0 CAPLUS
 CN Nickel, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



RN 42892-83-1 CAPLUS
 CN Nickel, dibromo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)

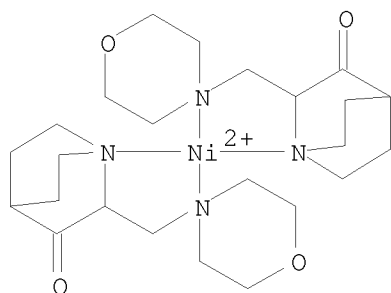


RN 42892-84-2 CAPLUS
 CN Nickel, diiodo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



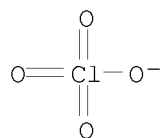
RN 42892-85-3 CAPLUS
 CN Nickel(2+), bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CRN 48228-23-5
 CMF C24 H40 N4 Ni O4
 CCI CCS

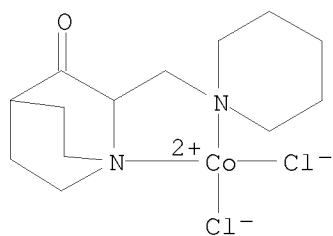


CM 2

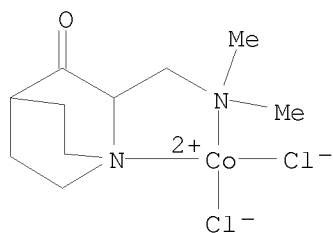
CRN 14797-73-0
 CMF C1 O4



RN 42892-86-4 CAPLUS
 CN Cobalt, dichloro[2-(1-piperidinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)

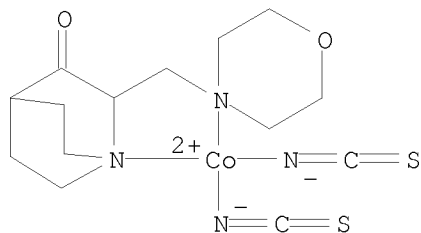


RN 42892-87-5 CAPLUS
 CN Cobalt, dichloro[2-[(dimethylamino)methyl]-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



RN 42942-73-4 CAPLUS

CN Cobalt, [2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



RN 43021-09-6 CAPLUS

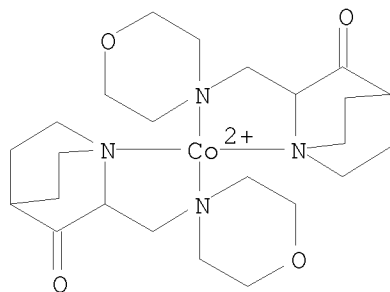
CN Cobalt(2+), bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 49857-57-0

CMF C24 H40 Co N4 O4

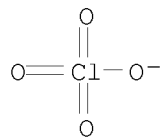
CCI CCS



CM 2

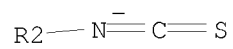
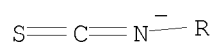
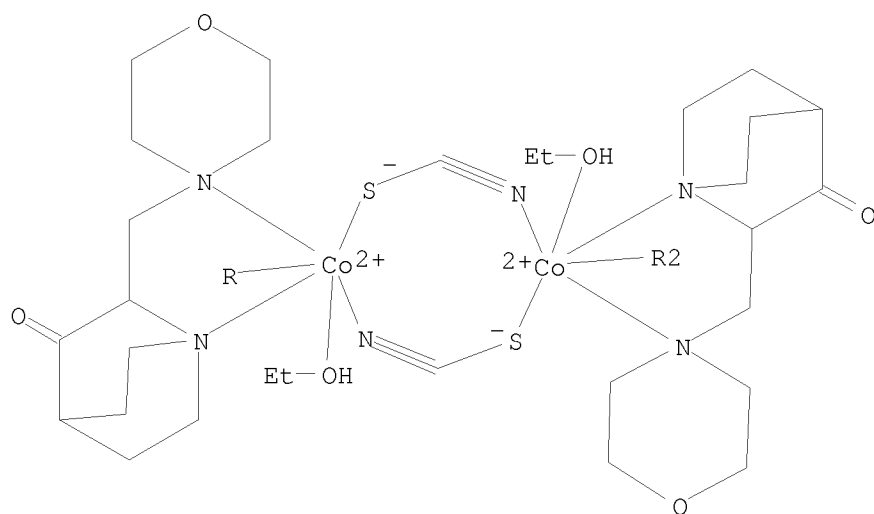
CRN 14797-73-0

CMF C1 O4

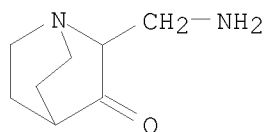


RN 54218-39-2 CAPLUS

CN Cobalt, bis(ethanol)bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]bis[μ-(thiocyanato-N:S)]bis(thiocyanato-N)di- (9CI) (CA INDEX NAME)



L15 ANSWER 102 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1973:499990 CAPLUS
 DOCUMENT NUMBER: 79:99990
 ORIGINAL REFERENCE NO.: 79:16163a,16166a
 TITLE: Selected first-row transition metal coordination
 compounds of 2-(N-aminomethyl)-3-quinuclidinone
 chelates
 AUTHOR(S): Dickinson, Richard C.
 CORPORATE SOURCE: Univ. Missouri, Rolla, MO, USA
 SOURCE: (1972) 118 pp. Avail.: Univ. Microfilms,
 Ann Arbor, Mich., Order No. 73-17,062
 From: Diss. Abstr. Int. B 1973, 34(1), 116
 DOCUMENT TYPE: Dissertation
 LANGUAGE: English
 AB Unavailable
 IT 42817-38-9DP, 1-Azabicyclo[2.2.2]octan-3-one, 2-(aminomethyl)-,
 transition metal complexes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 42817-38-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(aminomethyl)- (CA INDEX NAME)



L15 ANSWER 103 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:431939 CAPLUS
DOCUMENT NUMBER: 79:31939
ORIGINAL REFERENCE NO.: 79:5181a,5184a
TITLE: Amine-substituted 2-methylene-3-quinuclidones as
antibacterial agents
INVENTOR(S): Elkin, Samuel; Lieberman, Hillel
PATENT ASSIGNEE(S): Temple University
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3726877	A	19730410	US 1970-84927	19701028 <--

PRIORITY APPLN. INFO.: US 1970-84927 A 19701028

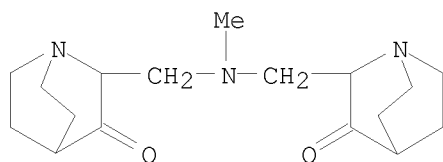
GI For diagram(s), see printed CA Issue.

AB About 30 title compds. (I, R = morpholino, Ph₂N, 2-isoquinolinyl, p-ClC₆H₄NH, o-MeC₆H₄NH, etc.) were prepared Thus, 2-methylene-3-quinuclidone was treated with morpholine to give I(R = morpholino). Several I were reduced to the corresponding alcs. I were antibacterial against Pseudomonas aeruginosa, Staphylococcus aureus, Escherichia coli, etc.

IT 19576-25-1P 41971-48-6P 41971-49-7P
41971-50-0P 41971-51-1P 41971-52-2P
41971-53-3P 41971-54-4P 41971-55-5P
41971-57-7P 41971-59-9P 41971-60-2P
41971-61-3P 41971-63-5P 41971-64-6P
41971-65-7P 41971-66-8P 41971-67-9P
41971-68-0P 41971-69-1P 41971-70-4P
41971-71-5P 41971-72-6P 41971-73-7P
42036-83-9P 42036-85-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

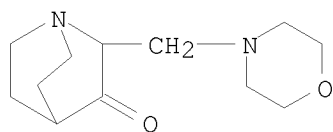
RN 19576-25-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis-(9CI) (CA INDEX NAME)



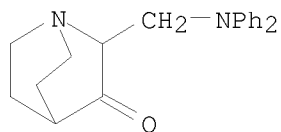
RN 41971-48-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



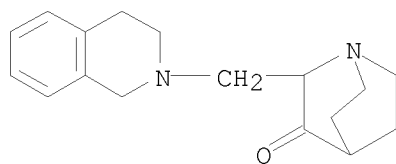
RN 41971-49-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(diphenylamino)methyl]- (CA INDEX NAME)



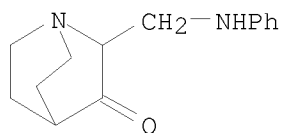
RN 41971-50-0 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]- (CA INDEX NAME)



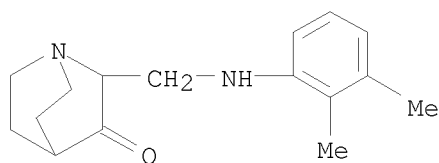
RN 41971-51-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylamino)methyl]- (CA INDEX NAME)



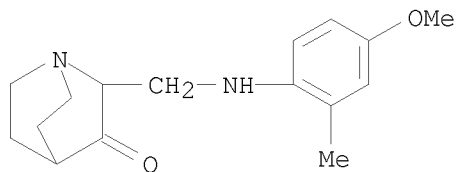
RN 41971-52-2 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,3-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



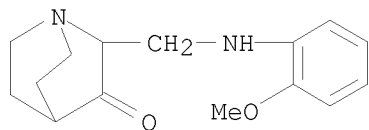
RN 41971-53-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-methoxy-2-methylphenyl)amino]methyl]- (CA INDEX NAME)



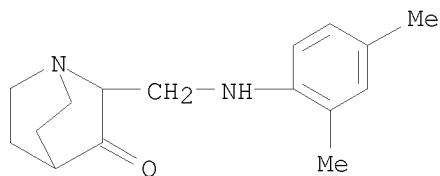
RN 41971-54-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methoxyphenyl)amino]methyl]- (CA INDEX NAME)



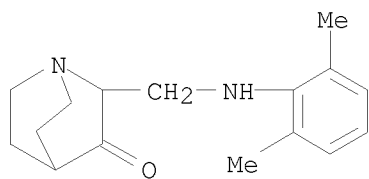
RN 41971-55-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,4-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



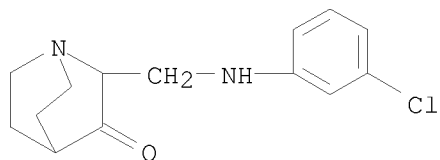
RN 41971-57-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,6-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



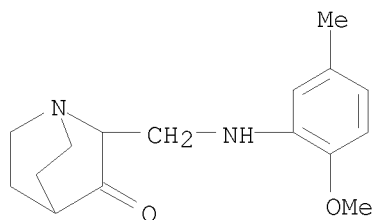
RN 41971-59-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(3-chlorophenyl)amino]methyl]- (CA INDEX NAME)

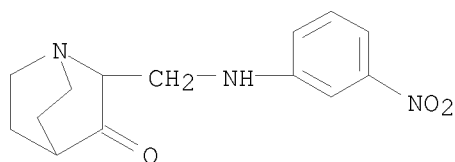


RN 41971-60-2 CAPLUS

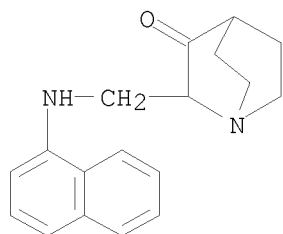
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methoxy-5-methylphenyl)amino]methyl]- (CA INDEX NAME)



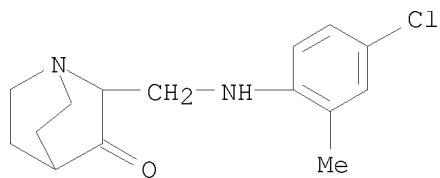
RN 41971-61-3 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[3-nitrophenyl]amino]methyl]- (CA INDEX NAME)



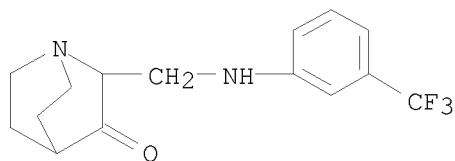
RN 41971-63-5 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(1-naphthalenylamino)methyl]- (CA INDEX NAME)



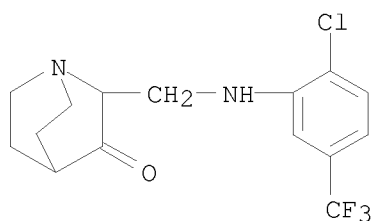
RN 41971-64-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-chloro-2-methylphenyl]amino]methyl]- (CA INDEX NAME)



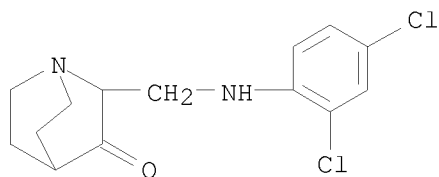
RN 41971-65-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[3-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



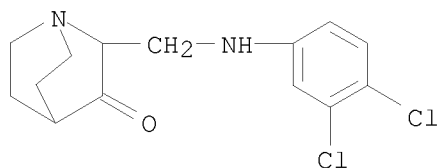
RN 41971-66-8 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



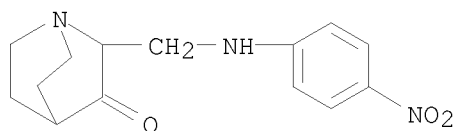
RN 41971-67-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



RN 41971-68-0 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[3,4-dichlorophenyl]amino]methyl]- (CA INDEX NAME)

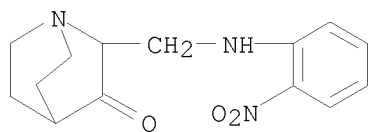


RN 41971-69-1 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[4-nitrophenyl]amino]methyl]- (CA INDEX NAME)



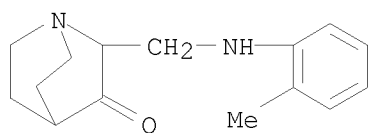
RN 41971-70-4 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-nitrophenyl)amino]methyl]- (CA INDEX NAME)



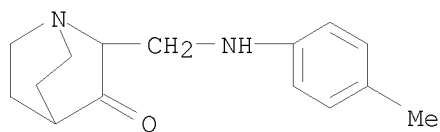
RN 41971-71-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methylphenyl)amino]methyl]- (CA INDEX NAME)



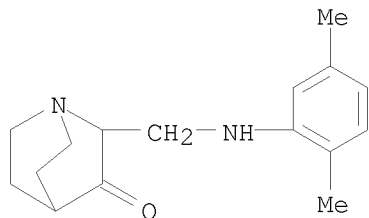
RN 41971-72-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-methylphenyl)amino]methyl]- (CA INDEX NAME)



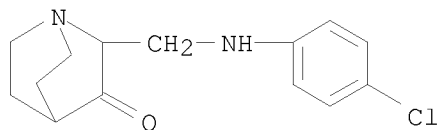
RN 41971-73-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,5-dimethylphenyl)amino]methyl]- (CA INDEX NAME)

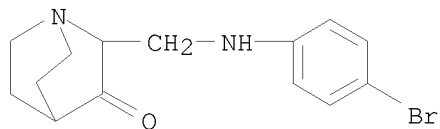


RN 42036-83-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-chlorophenyl)amino]methyl]- (CA INDEX NAME)



RN 42036-85-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-bromophenyl)amino]methyl]- (CA
INDEX NAME)



L15 ANSWER 104 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:431727 CAPLUS

DOCUMENT NUMBER: 79:31727

ORIGINAL REFERENCE NO.: 79:5145a,5148a

TITLE: Optically active triptycenes. VI. Optical resolution of 2,5-dihydroxy-8-methoxycarbonyltriptycene and absolute configuration of 2,5-dimethoxy-8-methoxycarbonyltriptycene

AUTHOR(S): Shimizu, Yasumi; Naito, Taketoshi; Ogura, Fumio; Nakagawa, Masazumi

CORPORATE SOURCE: Fac. Sci., Osaka Univ., Toyonaka, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(5), 1520-5

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

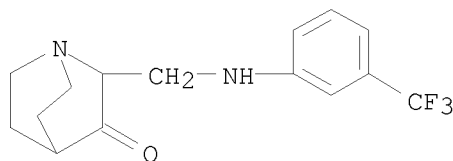
AB 2,5-Dihydroxy-8-(methoxycarbonyl)triptycene (I) was resolved via its dicamphanate derivative The absolute configuration of (+)-2,5-dimethoxy-8-(methoxycarbonyl)triptycene derived from I was (1R,6S) (by chemical correlation with (+)-2,5-dimethoxy-7-(dimethylamino)triptycene-HBr.

IT 41971-65-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 41971-65-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[3-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



L15 ANSWER 105 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:57263 CAPLUS

DOCUMENT NUMBER: 78:57263

ORIGINAL REFERENCE NO.: 78:9087a,9090a

TITLE: Use of mass spectrometry in structural and stereochemical studies. I. Mass spectra of β -quinuclidones and β -benzo(b)quinuclidones

AUTHOR(S): Ermakov, A. I.; Sheinker, Yu. N.; Mikhlin, E. E.; Mastafanova, L. I.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.; Kostyanovskii, R. G.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (10), 1404-10
CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

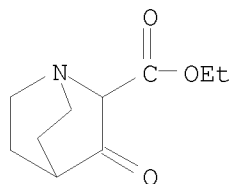
AB The mass spectra of β -quinuclidinones (I; R = H, Q = H₂, X = O; R = CO₂Me, Q = O, X = H₂; R = CO₂Et, Q = H₂, X = O; R = CO₂Et, Q = O, X = H₂) and benzo[b]quinuclidones (II; R = H, CO₂Et) were given. Labeling expts. indicated that fragmentation occurred by rupture of the bridge bond containing the keto group and subsequent loss of CO.

IT 34286-16-3

RL: PRP (Properties)
(mass spectrum of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



L15 ANSWER 106 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:551126 CAPLUS

DOCUMENT NUMBER: 77:151126

ORIGINAL REFERENCE NO.: 77:24839a,24842a

TITLE: PMR study of the tautomerism of 2-ethoxycarbonyl-3-oxoquinuclidine and -benzo [b] quinuclidine

AUTHOR(S): Turchin, K. F.; Sheinker, Yu. N.; Mikhлина, E. E.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im.

ORDZHONIKIDZE, Moscow, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (7), 978-83

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB 2-Ethoxycarbonyl-3-oxoquinuclidine existed primarily as the keto tautomer in nonpolar solvents, and as the N-protonated enolate in hydroxylic solvents; the lifetime of the individual forms in CD3OD at 75° was .apprx.0.3 sec. 2-Ethoxycarbonyl-3-oxobenzo-[b]quinuclidine existed as a mixture of syn and anti keto tautomers in CDCl3 and in CD3OD, with the syn diastereomer predominating; no enolic tautomers were observed The H at C-2 underwent D exchange in CD3OD at -24° (half life .apprx.2 min, activation energy .apprx.8 kcal/mol).

IT 34286-16-3

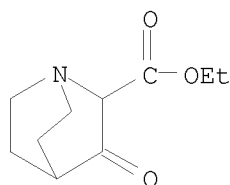
RL: PEP (Physical, engineering or chemical process); PRP (Properties);

PROC (Process)

(tautomerism of, NMR in relation to)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



L15 ANSWER 107 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:461774 CAPLUS
DOCUMENT NUMBER: 77:61774
ORIGINAL REFERENCE NO.: 77:10219a,10222a
TITLE: Michael reactions in the quinuclidin-3-one series
AUTHOR(S): Oppenheimer, Edna; Bergmann, Ernst D.
CORPORATE SOURCE: Dep. Chem., Heb. Univ., Jerusalem, Israel
SOURCE: Synthesis (1972), (5), 269-71
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

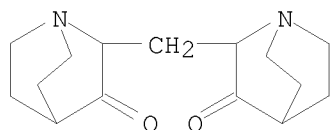
AB Enamine (I), prepared from 3-quinuclidinone (II, R = R1 = H) (III) and pyrrolidine, underwent Michael reaction with CH2:-CRCOMe (R = H, Me) to give the corresponding ethanoquinolines (IV); III gave II [RR1 = CHR2; R2 = H (V), Ph] with R2CHO, which were treated with (EtO2C)2CH2 in NaOEtHOEt to give II [R = H, R1 = (EtO2C)2CHCHR2; R2 = H (VI), Ph, resp.]. II (RR1 = PhCHMeCH, RR1 = Me2CHCH) were prepared analogously. V gave II [R = H, R1 = (EtO2C)2CHCHR2; R2 = NHAc] (VII) with AcNHCH(CO2Et)2. VI and VII were hydrolyzed with HCl-HOAc to II [R = H, R1 = HO2C(CH2)2; R = H, R1 = HO2CCH(NH2)CH2], resp.

IT 37040-83-8P 37040-87-2P 37040-88-3P
37040-89-4P 37040-90-7P 37395-64-5P
37395-65-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

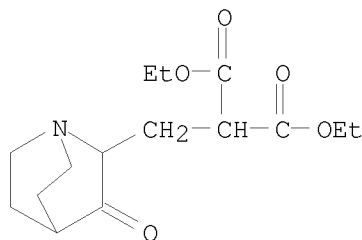
RN 37040-83-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-methylenebis- (CA INDEX NAME)



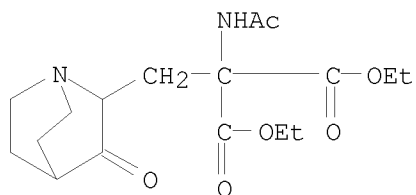
RN 37040-87-2 CAPLUS

CN Propanedioic acid, [(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



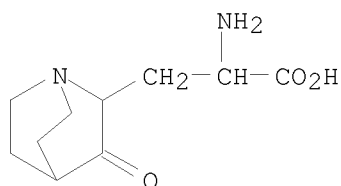
RN 37040-88-3 CAPLUS

CN Propanedioic acid, (acetylamino)[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 37040-89-4 CAPLUS

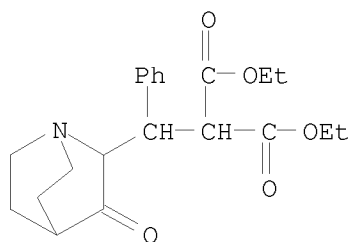
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, α -amino-3-oxo-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

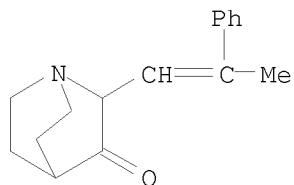
RN 37040-90-7 CAPLUS

CN Propanedioic acid, [(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)phenylmethyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 37395-64-5 CAPLUS

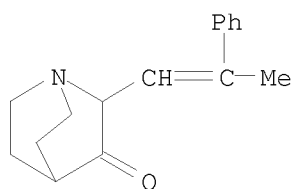
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(2-phenyl-1-propenyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 37395-65-6 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(2-phenyl-1-propenyl)- (9CI) (CA INDEX
NAME)



L15 ANSWER 108 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:404638 CAPLUS

DOCUMENT NUMBER: 77:4638

ORIGINAL REFERENCE NO.: 77:830h,831a

TITLE: Tautomerism of 2-ethoxycarbonyl-3-Oxo derivatives of quinuclidine and benzo[b]quinuclidine

AUTHOR(S): Sheinker, Yu. N.; Peresleni, E. M.; Persianova, I. V.; Mikhlina, E. E.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (2), 229-33

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Using ir and uv spectroscopy and potentiometric titration existence of 2-ethoxycarbonyl-3-oxoquinuclidine in the keto, enol, and zwitterionic forms was established. The tautomeric equilibrium was affected by the aggregate state (concentration) and by the solvent nature. In the crystalline state

and in polar solvents the zwitterionic form prevailed, in nonpolar solvents existence of keto and enol forms was proved.

-Ethoxycarbonyl-3-oxobenzo [b]quinuclidine existed in the keto form in al

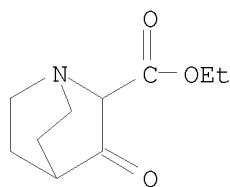
IT 34286-16-3 37832-15-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(tautomerism of, ir spectrum in relation to)

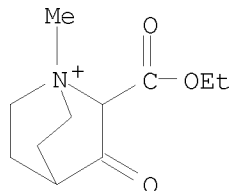
RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 37832-15-8 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 2-(ethoxycarbonyl)-1-methyl-3-oxo-, iodide (9CI) (CA INDEX NAME)



● I⁻

L15 ANSWER 109 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:140119 CAPLUS

DOCUMENT NUMBER: 76:140119

ORIGINAL REFERENCE NO.: 76:22727a,22730a

TITLE: Hydrogen transfer from formyl compounds to α,β -unsaturated ketones catalyzed by ruthenium, rhodium, and iridium complexes

AUTHOR(S): Blum, Jochanan; Sasson, Yoel; Iflah, Shulah

CORPORATE SOURCE: Dep. Org. Chem., Heb. Univ., Jerusalem, Israel

SOURCE: Tetrahedron Letters (1972), (11), 1015-18

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

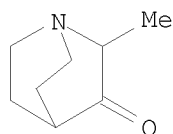
AB Phenethyl ketones $\text{PhCH}_2\text{CH}_2\text{COR}$ (I, R = Ph, CMe₃ and Me) were prepared by transfer-hydrogenation of PhCH:CHCOR using α -naphthaldehyde, p-MeC₆H₄CHO, HCONHMe or HCO₂H as H donors in the presence of catalytic amts. of (Ph₃P)₃RuCl₂, (Ph₃P)₃RhCl or (Ph₃P)₂IrCl(CO). The transferred H atoms are derived exclusively from the formyl group. HCO₂H was an excellent H donor and gave 94-6% yields of the ketones. Side reactions due to decarbonylation of the aldehydes and condensation of the ketones were also present. BuPh in 10% yield was obtained by reducing $\text{PhCH}_2\text{CH}_2\text{CH:CH}_2$ with HCO₂H.

IT 5291-14-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5291-14-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)



L15 ANSWER 110 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

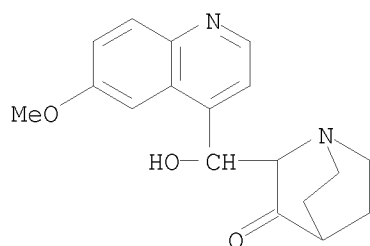
ACCESSION NUMBER: 1972:46360 CAPLUS
DOCUMENT NUMBER: 76:46360
ORIGINAL REFERENCE NO.: 76:7480h,7481a
TITLE: Synthetic quinine analogs. V. Quinolinemethanols related to devinylquinine
AUTHOR(S): Bender, D. R.; Coffen, D. L.
CORPORATE SOURCE: Dep. Chem., Univ. Colorado, Boulder, CO, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(6), 937-42
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:46360

AB Aldol condensation of quin-olinecarboxaldehydes with 3-quinuclidinone followed by acid-catalyzed hydration of the resulting α,β -unsatd. ketones provides a short and versatile synthesis of devinylquinine derivs. A novel rearrangement of 2-(9-phenanthrylmethylene)-3-quinuclidinyl carbinols leading to dibenzindole derivs. is described.

IT 35722-03-3P 35839-90-8P 35839-91-9P
35845-49-9P 35845-54-6P 35870-57-6P
35870-58-7P 36468-36-7P 36547-75-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

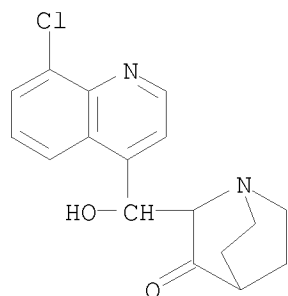
RN 35722-03-3 CAPLUS

CN 10,11-Dinorcinchonane-7-one, 9-hydroxy-6'-methoxy-, (8 α)-(±)-
(9CI) (CA INDEX NAME)



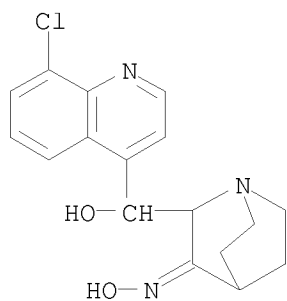
RN 35839-90-8 CAPLUS

CN 10,11-Dinorcinchonane-7-one, 8'-chloro-9-hydroxy-, (8 α)-(±)- (9CI)
(CA INDEX NAME)

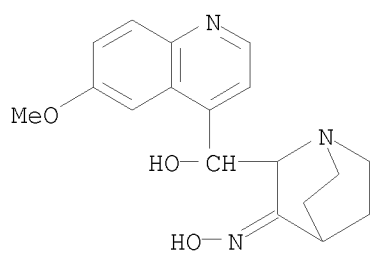


RN 35839-91-9 CAPLUS

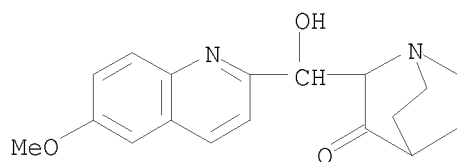
CN 10,11-Dinorcinchonane-7-one, 8'-chloro-9-hydroxy-, oxime,
(8 α)-(±)- (9CI) (CA INDEX NAME)



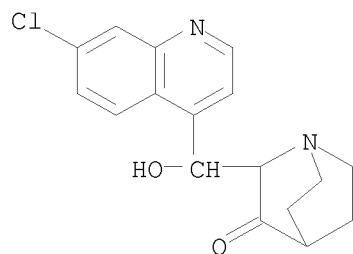
RN 35845-49-9 CAPLUS
 CN 10,11-Dinorcinchonan-7-one, 9-hydroxy-6'-methoxy-, oxime,
 (8 α)-(±)-(9CI) (CA INDEX NAME)



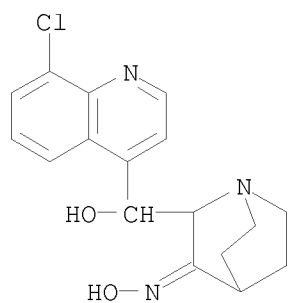
RN 35845-54-6 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[hydroxy(6-methoxy-2-quinolinyl)methyl]-
 (CA INDEX NAME)



RN 35870-57-6 CAPLUS
 CN 10,11-Dinorcinchonan-7-one, 7'-chloro-9-hydroxy-, (8 α)-(±)-(9CI)
 (CA INDEX NAME)

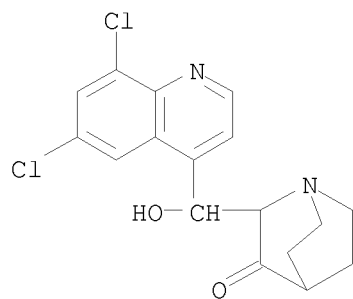


RN 35870-58-7 CAPLUS
 CN 10,11-Dinorcinchonan-7-one, 8'-chloro-9-hydroxy-, oxime, hydrochloride,
 (8 α)-(±)-(9CI) (CA INDEX NAME)

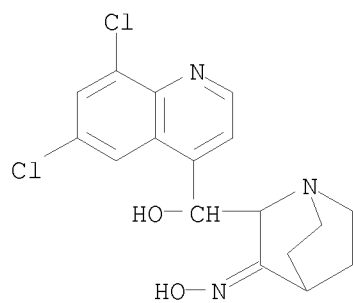


●_x HCl

RN 36468-36-7 CAPLUS
 CN 10,11-Dinorcinchonane-7-one, 6',8'-dichloro-9-hydroxy-, (8 α)-(±)-
 (9CI) (CA INDEX NAME)



RN 36547-75-8 CAPLUS
 CN 10,11-Dinorcinchonane-7-one, 6',8'-dichloro-9-hydroxy-, oxime,
 (8 α)-(±)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1972:45521 CAPLUS
 DOCUMENT NUMBER: 76:45521
 ORIGINAL REFERENCE NO.: 76:7349a,7352a
 TITLE: Effect of transition-state geometry on the
 [2,3]-sigmatropic rearrangements of ammonium ylides
 AUTHOR(S): Mageswaran, S.; Ollis, W. D.; Sutherland, I. O.;
 Thebtaranonth, Y.
 CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, UK
 SOURCE: Journal of the Chemical Society [Section] D: Chemical
 Communications (1971), (22), 1494-5
 CODEN: CCJDAO; ISSN: 0577-6171

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The ylides (I, R=PhCH₂, PhCH:CHCH₂) prepared from 1-benzyl- and
 1-(cinnamyl)-1-azoniabicyclo[2.2.2]octan-3-one bromides by treatment with
 aqueous NaOH did not undergo [2,3]-sigmatropic rearrangements cleanly but gave
 complex mixts. of products. The less strained ylide (II, R=PhCH:CHCH₂)
 generated by base from a 1-(cinnamyl)-1-azoniabicyclo[3.3.1]nonan-3-one
 salt gave at 120° 85% of the [2,3]-sigmatropically rearranged
 product, 2-(1-phenyl-2-propenyl)-1-azabicyclo[3.3.1]nonan-3-one.

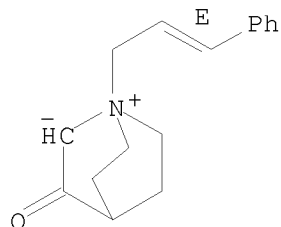
IT 79841-03-5 79841-04-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (pyrolysis of)

RN 79841-03-5 CAPLUS

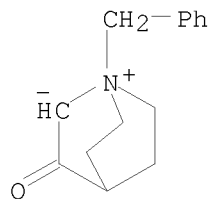
CN 1-Azoniabicyclo[2.2.2]octane, 3-oxo-1-(3-phenyl-2-propenyl)-, ylide, (E)-
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 79841-04-6 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-oxo-1-(phenylmethyl)-, ylide (9CI) (CA
 INDEX NAME)



L15 ANSWER 112 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:551255 CAPLUS

DOCUMENT NUMBER: 75:151255

ORIGINAL REFERENCE NO.: 75:23853a,23856a

TITLE: Stereochemistry of benzo[b]quinuclidines. I.

Determination of the configuration of 3- and

2,3-substituted benzo[b]quinuclidines by PMR

AUTHOR(S):

Turchin, K. F.; Mikhлина, E. E.; Yanina, A. D.;

Vorob'eva, V. Ya.; Yakhontov, L. N.; Sheinker, Yu. N.

CORPORATE SOURCE:

Vses. Nauchno-Issled. Khim.-Farm. Inst. im.

Ordzhonikidze, Moscow, USSR

SOURCE:

Khimiya Geterotsiklicheskikh Soedinenii (1971

), 7(7), 981-6

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

AB Observed trends in changes of chemical shifts and spin-spin coupling consts. of the quinuclidine unit protons owing to substitution in 2- and 3-positions of benzo[b]quinuclidine permit determination of syn and anti orientations (to

the

attached benzene ring) of protons in 2- and 3-positions in the title compds.

IT 34286-16-3

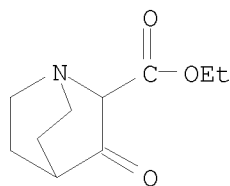
RL: PRP (Properties)

(nuclear magnetic resonance of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA

INDEX NAME)



L15 ANSWER 113 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:550911 CAPLUS

DOCUMENT NUMBER: 75:150911

ORIGINAL REFERENCE NO.: 75:23801a,23804a

TITLE: Mass spectra of β -quinuclidones and β -benzoquinuclidones

AUTHOR(S): Ermakov, A. I.; Sheinker, Yu. N.; Mikhлина, E. E.; Mastafanova, L. I.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhnotov, L. N.; Kostyanovskii, R. G.

CORPORATE SOURCE: S. Ordzhonikidze All Union Chem.-Pharm. Res. Inst., Moscow, USSR

SOURCE: Organic Mass Spectrometry (1971), 5(9), 1029-41

CODEN: ORMSBG; ISSN: 0030-493X

DOCUMENT TYPE: Journal

LANGUAGE: English

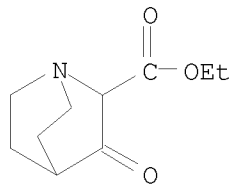
AB The mass spectra of quinuclid-3-one, benzoquinuclid-3-one, 2-azaquinuclid-3-one, 2-azabenzquinuclid-3-one and some of their functional substituted derivs. were investigated. Fragmentation of the compds. investigated proceeded through the open form of the mol. ion with cleavage of a bridgehead bond containing the carbonyl group and subsequent elimination of CO.

IT 34286-16-3 34291-64-0 34291-65-1
34291-66-2

RL: PRP (Properties)
(mass spectrum of)

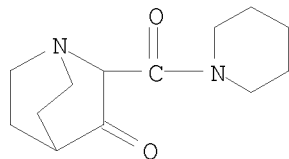
RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



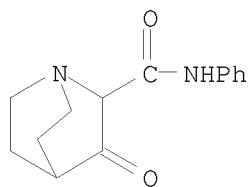
RN 34291-64-0 CAPLUS

CN Piperidine, 1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



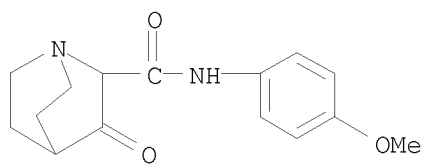
RN 34291-65-1 CAPLUS

CN 2-Quinuclidinecarboxanilide, 3-oxo- (8CI) (CA INDEX NAME)



RN 34291-66-2 CAPLUS

CN 2-Quinuclidinecarbox-p-anisidide, 3-oxo- (8CI) (CA INDEX NAME)

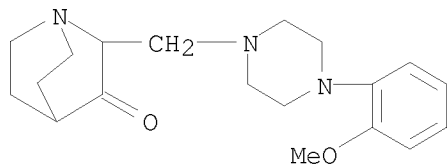


L15 ANSWER 114 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

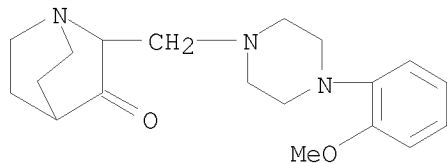
ACCESSION NUMBER: 1971:510339 CAPLUS
DOCUMENT NUMBER: 75:110339
ORIGINAL REFERENCE NO.: 75:17427a,17430a
TITLE: 2-[N-(o-alkoxyphenyl)piperazinomethyl]-3-quinuclidinones as tranquilizers and central nervous system depressants in mammals
INVENTOR(S): Biel, John H.; Hopps, Harvey B.
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3598825	A	19710810	US 1967-690087	19671213 <--
PRIORITY APPLN. INFO.:			US 1967-690087	A 19671213

GI For diagram(s), see printed CA Issue.
AB The substituted quinuclidinones (I, R = lower alkyl) are prepared by reacting an N-(o-alkoxyphenyl)piperazine with 2-methylene-3-quinuclidinone (II) in a suitable solvent at 20-100°. Mannich reaction of 3-quinuclidinone with Me₂NH and CH₂O in absolute alc. and heating the Mannich base intermediate at reflux temperature yields II by spontaneous deamination. Thus, II and N-(o-methoxyphenyl)piperazine in MeOH kept 60 hr at 20° yielded 63% I (R = Me), m. 108.5-9.5°. Similarly were obtained I (R = Et, Pr, iso-Pr, Bu, CMe₃, C₅H₁₁).
IT 33606-15-4P 33606-16-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33606-15-4 CAPLUS
CN 3-Quinuclidinone, 2-[[4-(o-methoxyphenyl)-1-piperazinyl]methyl]- (8CI)
(CA INDEX NAME)



RN 33606-16-5 CAPLUS
CN 3-Quinuclidinone, 2-[[4-(o-methoxyphenyl)-1-piperazinyl]methyl]-, trihydrochloride (8CI) (CA INDEX NAME)



L15 ANSWER 115 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:405735 CAPLUS
DOCUMENT NUMBER: 75:5735
ORIGINAL REFERENCE NO.: 75:951a,954a
TITLE: 2-Benzhydrylquinuclidines as diuretics
INVENTOR(S): Warawa, Edward J.
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3560510	A	19710202	US 1969-804691	19690305 <--
PRIORITY APPLN. INFO.:			US 1969-804691	A 19690305

GI For diagram(s), see printed CA Issue.

AB Cis and trans isomers of the title compds. are obtained by isolating the cis or trans isomer from a mixture of cis,trans-2-benzhydryl-3-(benzylamino)quinuclidines by chromatog. and subsequent catalytic debenzylation. Alternatively, a mixture of cis,trans-3-amino analog is acetylated with Ac2O and the 3-acetamido derivs. separated by fractional crystallization from iso-PrOH and hydrolyzed in concentrated HCl. BzH reacted with

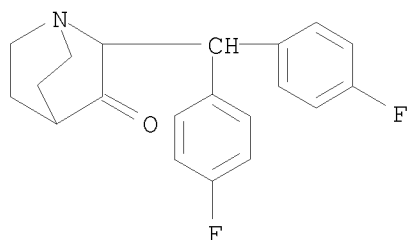
3-quinuclidinone in alc. in the presence of a base, the 2-benzylidene-3-quinuclidinone treated with PhMgBr in Et2O-C6H6, the resultant 2-benzhydryl-3-quinuclidinone distilled azeotropically with PhCH2NH2 in PhMe in the presence of p-MeC6H4SO3H, and the 2-benzhydryl-3-(benzylimino)quinuclidine reduced with NaBH4 yielded pure cis-I.

IT 24802-69-5P 24802-70-8P 32531-66-1P
32531-67-2P 32531-68-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

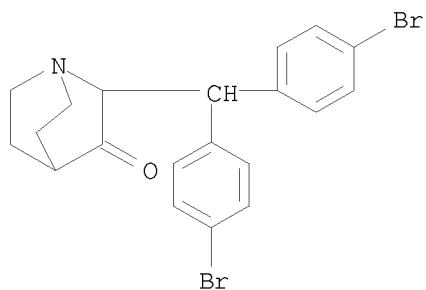
RN 24802-69-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-fluorophenyl)methyl]- (CA INDEX NAME)

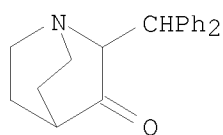


RN 24802-70-8 CAPLUS

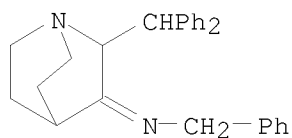
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-bromophenyl)methyl]- (CA INDEX NAME)



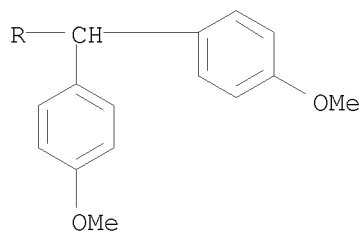
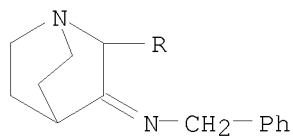
RN 32531-66-1 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(diphenylmethyl)- (CA INDEX NAME)



RN 32531-67-2 CAPLUS
 CN Benzenemethanamine, N-[2-(diphenylmethyl)-1-azabicyclo[2.2.2]oct-3-ylidene]- (CA INDEX NAME)



RN 32531-68-3 CAPLUS
 CN Benzenemethanamine, N-[2-[bis(4-methoxyphenyl)methyl]-1-azabicyclo[2.2.2]oct-3-ylidene]- (CA INDEX NAME)



L15 ANSWER 116 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:487840 CAPLUS

DOCUMENT NUMBER: 73:87840

ORIGINAL REFERENCE NO.: 73:14357a,14360a

TITLE: Synthesis and properties of 3-hydroxypyrazolo[4,3-b]quinuclidine

AUTHOR(S): Mikhlina, E. E.; Vorob'eva, V. Ya.; Turchin, K. F.; Kostyuchenko, N. P.; Sheinker, Yu. N.; Yakhontov, L. N.

CORPORATE SOURCE: Vses. Nauch.-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1970), (5), 651-6

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

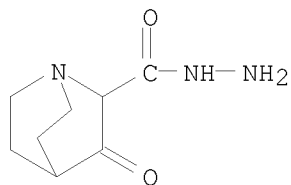
AB The influence of the quinuclidine system on the third condensed ring was studied. The mixture of 3 g 2-carbethoxy-3-oxoquinuclidine (I), 12 ml EtOH, and 2 g N₂H₄ reacts at room temperature 3 hr, to form, 96% 3-oxoquinuclidine-2-carboxylic acid hydrazide (II), which decomp. to 72% 3-hydroxypyrazolo[4,3-b]quinuclidine (III), m. 290.5°, when dissolved in boiling water. The yield increases to 98-9% after prolonged boiling or after heating in vacuo. III was also obtained directly from I and N₂H₄ at higher temps. III.HCl m. 208-10°; III.2HCl m. 199-200°; III.Ag salt m. 238° (decomposition). Methylation of III with Me₂SO₄ yielded its 2-Me derivative, m. 222-4°; hydrochloride m. 248-50°. Treatment of 1 mole III with 1 or 2 moles BzCl, resp., gives 61.3% 1-Bz derivative, m. 205-7°, or 84.5% 1-Bz derivative of the 3-benzoate of III, m. 148-50°. III reacts with acrylonitrile under reflux to form 36.8% 1-(β-cyanoethyl) derivative of III, m. 222-3.5°. Reaction of III with boiling Ac₂O yields 56% 1-acetyl derivative of the 3-acetate of III, m. 127-8°; hydrochloride m. 214-17°; 1-acetyl derivative of III, m. 212-14°, was obtained by saponifying the 3-acetate or by treatment with Ac₂O-pyridine mixture at room temperature. Similarly to III, 44% methylhydrazide of 3-oxoquinuclidine-2-carboxylic acid (IV), m. 227-30°, was prepared from 3 g I and a solution of 2.44 g NaOH and 4.38 g methylhydrazine sulfate in 20 ml EtOH. IV heated gave 98% 1-Me derivative of III, m. 244°; dihydrochloride m. 194-7° (decomposition).

IT 28710-66-9P 28710-77-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

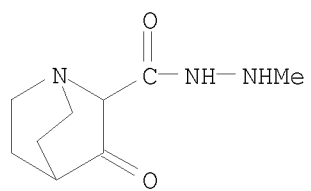
RN 28710-66-9 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, hydrazide (8CI) (CA INDEX NAME)

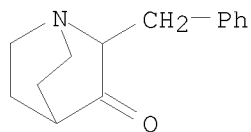


RN 28710-77-2 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, 2-methylhydrazide (8CI) (CA INDEX NAME)



L15 ANSWER 117 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1970:487765 CAPLUS
 DOCUMENT NUMBER: 73:87765
 ORIGINAL REFERENCE NO.: 73:14341a,14344a
 TITLE: Preparation of 3,4,4a,5,11,11a-hexahydro-1,4-ethano-1H-benzo[5,6]cyclohepta[1,2-b]pyridin-6-(2H)one
 AUTHOR(S): Villani, Frank J.; Wefer, Elizabeth A.
 CORPORATE SOURCE: Dep. of Med. Chem., Schering Co., Bloomfield, NJ, USA
 SOURCE: Journal of Heterocyclic Chemistry (1970), 7(4), 973-4
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 73:87765
 GI For diagram(s), see printed CA Issue.
 AB The title compound (I) is prepared by the cyclization of 2-benzyl-3-carboxymethylquinuclidine (II) with polyphosphoric acid or by the treatment of II acid chloride with AlCl₃. 2-Benzylidene-3-quinuclidinone (III) is converted to the 2-benzyl derivative, which is treated with Et (diethylphosphono)acetate, and reduced to give II.
 IT 28281-22-3P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 28281-22-3 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(phenylmethyl)- (CA INDEX NAME)



L15 ANSWER 118 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:456081 CAPLUS
DOCUMENT NUMBER: 73:56081
ORIGINAL REFERENCE NO.: 73:9217a,9220a
TITLE: Analgesic 2,3-heterocyclic fused quinuclidines and
3-substituted quinuclidine-2-carboxylate derivatives
INVENTOR(S): Remers, William A.; Gibbs, Gabriel J.; Weiss, Martin J.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 3501471	A	19700317	US 1966-580894	19660921 <--
PRIORITY APPLN. INFO.:			US 1966-580894	A 19660921

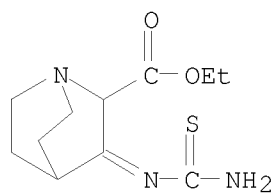
GI For diagram(s), see printed CA Issue.

AB The title compds. (I, where XYZ = pyrazolino, pyridazolino, pyrimidino, triazolino, or isoxazolino fusions) are central nervous system depressants and analgesic. Et 3-quinuclidinone-2-carboxylate-HCl (II) (7 g) and 25 ml N₂H₄.H₂O was refluxed 16 hr and the product treated with 30 ml N HCl to yield pyrazol[3]ino[4,3-b]quinuclidin-3-one-HCl, m. 213-16°. Similarly, II and MeNHNH₂ gave 2-methylpyrazol[3]ino[4,3-b]quinuclidin-3-one, m. 217-20° (CH₂Cl₂-n-C₆H₁₄). II (7 g), 2.9 g guanidine-HCl, and 60 ml EtOH was refluxed 2 hr to yield Et 2,3-didehydro-3-guanidinoquinuclidine-2-carboxylate-2HCl.H₂O, m. 179-81°, which with EtONa in EtOH gave 2-amino-3H-pyrimidino[5,4-b]quinuclidin-4-one guanidinate hemihydrate, m. 258° (EtOH). II and thiourea was refluxed 24 hr in EtOH to yield Et 3-thiocarbamoyliminoquinuclidine-2-carboxylate-HCl.EtOH. 2,3-Didehydroquinuclidine-2,3-dicarboxylic acid was treated with AcCl and Ac₂O to give the anhydride, which with anhydrous NH₃ in THF gave 2,3-didehydroquinuclidine-2,3-dicarboxylic acid imide. 2,3-Didehydroquinuclidine, and PhN₃ gave 1-phenyl-v-triazol[2]ino[4,5-b]-quinuclidine, m. 160-3°. Me 2,3-didehydroquinuclidine-3-carboxylate (III) (0.84 g), 1.6 g N-(α-chlorobenzylidene)-N'-phenylhydrazine, and 25 ml THF was treated with 0.81 g Et₃N in 10 ml THF the product treated with HCl to give Me 2,7-diphenylpyrazol[5]ino[3,4-b]quinuclidine-6a-carboxylate-HCl, m. 223-35°. III and Ph₃N gave Me 3-phenyl-v-triazol[1]ino[4,5-b]quinuclidine-7a-carboxylate, m. 143.5-5.5°.

IT 27952-10-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27952-10-9 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-[(thiocarbamoyl)imino]-, ethyl ester, hydrochloride (8CI) (CA INDEX NAME)

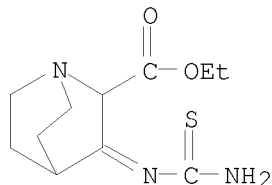


●_x HCl

L15 ANSWER 119 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:435237 CAPLUS
DOCUMENT NUMBER: 73:35237
ORIGINAL REFERENCE NO.: 73:5837a,5840a
TITLE: Analgesic 2,3-heterocyclic fused quinuclidines and
3-substituted quinuclidine-2-carboxylate derivatives
INVENTOR(S): Remers, William A.; Gibbs, Gabriel J.; Weiss, Martin J.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

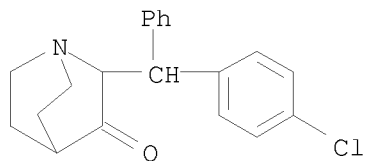
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	US 3501471		19700317	US	19660921 <--
GI	For diagram(s), see printed CA Issue.				
AB	Title compds., useful as central nervous system depressants and analgesic agents, were prepared Thus, 7 g Et 3-quinuclidinone-2-carboxylate-HCl hydrochloride (I) and 25 ml N2H4.H2O was refluxed 16 hr, to yield pyrazol[3]ino[4,3-b]quinuclidin-3-one-HCl, m. 213-16°. Similarly, I and MeNH-NH2 gave 2-methylpyrazol[3]ino[4,3-b]quinuclidin-3-one (II), m. 217-20° (CH2Cl2-n-C6H14). I (7 g), 2.9 g guanidine-HCl, and 60 ml EtOH was refluxed 2 hr to yield Et 2,3-dehydro-3-guanidinoquinuclidine-2-carboxylate-2HCl.H2O, m. 179-81°, which treated with EtONa in EtOH gave 2-amino-3H-pyrimidino[5,4-b]quinuclidin-4-one guanidinate-0.5H2O, m. 258° (EtOH). I and thiourea was refluxed 24 hr in EtOH to yield Et 3-thiocarbamoyliminoquinuclidine-2-carboxylate-HCl alcoholate, yellow glassy solid. 2,3-Dehydroquinuclidine-2,3-dicarboxylic acid was treated with AcCl and Ac2O to give the anhydride, oil, which was converted with anhydrous NH3 in THF into 2,3-dehydroquinuclidine-2,3-dicarboxylic acid imide, white solid. 2,3-Dehydroquinuclidine and PhN3 gave 1-phenyl-v-triazol[2]ino[4,5-b]quinuclidine, m. 160-3°. Me 2,3-dehydroquinuclidine-3-carboxylate (III) (0.84 g), 1.6 g N-(α-chlorobenzylidene)-N'-phenylhydrazine, and 25 ml THF was cooled in an ice bath, treated with 0.81 g Et3N in 10 ml THF, and the mixture kept 16 hr to give Me 2,7-diphenylpyrazol[5]ino-[3,4-b]quinuclidine-6a-carboxylate-HCl, m. 223-35°. III and Ph3N gave Me 3-phenyl-v-triazol[1]ino[4,5-b]quinuclidine-7a-carboxylate, m. 143.5-5.5°.				
IT	27952-10-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	27952-10-9 CAPLUS				
CN	2-Quinuclidinecarboxylic acid, 3-[(thiocarbamoyl)imino]-, ethyl ester, hydrochloride (8CI) (CA INDEX NAME)				



●x HCl

L15 ANSWER 120 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1970:403814 CAPLUS
 DOCUMENT NUMBER: 73:3814
 ORIGINAL REFERENCE NO.: 73:649a,652a
 TITLE: 2-[4'-(Chloro)-benzylidryl]-3-quinuclidinols as central
 nervous system stimulants
 INVENTOR(S): Warawa, Edward J.; Mueller, Nancy Jean
 PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
 SOURCE: U.S., 4 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3506673	A	19700414	US 1968-717405	19680329 <--
PRIORITY APPLN. INFO.:			US 1968-717405	A 19680329
GI	For diagram(s), see printed CA Issue.			
AB	A grignard reagent was prepared from 25.1 g PhBr in 200 ml anhydrous Et ₂ O, 4.28 g Mg turnings and a trace of iodine; after refluxing 2.5 hr and cooling (ice bath), a solution of 26.52 g 2-(4-chlorobenzylidenyl)-3-quinuclidinone in 400 ml C ₆ H ₆ was added dropwise over 3.75 hr, and the mixture stirred overnight at room temperature crystallized from alc. to give 44.8% 2-(4-chlorobenzhydryl)-3-quinuclidinone (I) m. 145-80°. A soln of 1 g I, 3.5 g (iso-PrO) ₃ Al, and 20 ml anhydrous iso-PrOH was heated on a steam bath while N was slowly passed in 2.5 hr, then worked up to give the corresponding alc., (50:50 mixture of the cis isomers containing a trace of trans isomer) separated by chromatog. to give 330 mg α-cis isomer, m. 169-70.5° (MeOH); 250 mg mixt of α-and β-isomers; and 350 mg β-cis isomer, m. 236-6.5° (decomposition) (MeOH).			
IT	27655-54-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	27655-54-5 CAPLUS			
CN	1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-chlorophenyl)phenylmethyl]- (CA INDEX NAME)			



L15 ANSWER 121 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:31644 CAPLUS
DOCUMENT NUMBER: 72:31644
ORIGINAL REFERENCE NO.: 72:5785a,5788a
TITLE: 2-(4,4'-Difluoro- and 2-(4,4'-dibromobenzhydryl)-3-quinuclidinol
INVENTOR(S): Warawa, Edward J.; Mueller, Nancy Jean
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: Ger. Offen., 31 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1915142	A	19691002	DE 1969-1915142	19690325 <--
US 3506672	A	19700414	US 1968-717389	19680329 <--
NL 6904655	A	19691001	NL 1969-4655	19690326 <--
GB 1257387	A	19711215	GB 1969-1257387	19690326 <--
DK 122128	B	19720124	DK 1969-1657	19690326 <--
BE 730701	A	19690929	BE 1969-730701	19690328 <--
FR 2005129	A5	19691205	FR 1969-9467	19690328 <--
CH 499520	A	19701130	CH 1969-499520	19690328 <--
			US 1968-717389	A 19680329

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

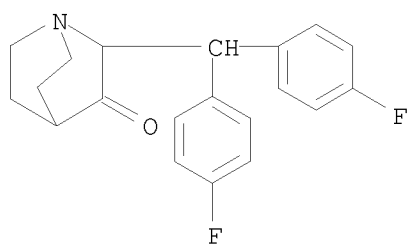
AB The title products (I), for the treatment of arthritis, rheumatism, and other inflammations, are prepared by reacting 3-quinuclidone (II) with p-fluorobenzaldehyde (III) or p-bromobenzaldehyde to give 2-(4-fluoro)benzylidene-3-quinuclidone (IV) or the Br analog, which is treated with p-BrC₆H₄F or p-Br₂C₆H₄ in a Grignard reaction to give 2-(4,4'-difluorobenzhydryl)-3-quinuclidone (V), which is reduced with Al isopropoxide to give (±)-cis-I (X = F) or with NaBH₄ to give a mixture of cis- and trans-I, which is repeatedly oxidized with Ph₂CO and again reduced with NaBH₄ until pure trans-I is obtained. Thus, 12.5 g. II, 12.4 g III, and 1 pellet NaOH in 25 ml EtOH was refluxed 2.5 hr to give 20.9 g. IV, m. 118.5-20.5°. To 175 g p-BrC₆H₄F, 26.7 g Mg, and a trace of iodine in 900 ml Et₂O was added 151 g IV in 19 l. benzene in 6.5 hr to give 143.1 g V, m. 160-2.5°. V (120 g) and 200 g Al isopropoxide in iso-PrOH gave 98.16 g (±)-cis-I (X = F), m. 197-8° (MeOH), HCl salt m. 297-300°. Salts were prepared with (-)-mandelic acid and with (±)-mandelic acid; the optically active mandelates m. 228-30°; from these were made (+)-cis-I, m. 185-6°, [α]_D²⁵ 20° and its antipode, [α]_D²⁵ -20°, m. 185-6°. The optically active HCl salts have [α]_D²⁵ 27° and -27°. IV (5 g) in 175 ml EtOH and 25 ml CH₂Cl₂ was treated with 1.16 g. NaBH₄ to give 5.31 g mixture of (±)-cis- and trans-I. This was treated in 45 ml benzene with 11.56 g Ph₂CO and 1.42 g KH in 35 ml benzene and refluxed 0.75 hr to give 4.69 g mixed trans-I (X = F) and IV, which was reduced with NaBH₄ as above. The whole process was repeated twice to obtain 0.85 g (±)-trans-I, m. 190-2°. Similarly was obtained 84.5% 2-(4-bromo)benzylidene-3-quinuclidone, m. 125-6°, and from this 32% 2-(4,4'-dibromobenzhydryl)-3-quinuclidone, m. 191-3°; this gave on reduction with Al isopropoxide 68.3% (±)-cis-I (X = Br), m. 205-6°.

IT 24802-69-5P 24802-70-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

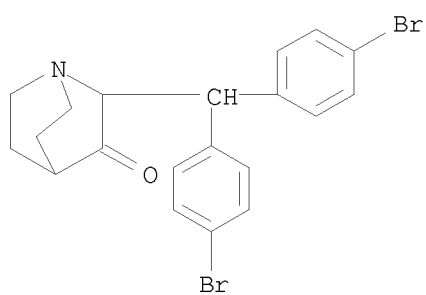
RN 24802-69-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-fluorophenyl)methyl]- (CA INDEX NAME)



RN 24802-70-8 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-bromophenyl)methyl]- (CA INDEX NAME)



L15 ANSWER 122 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:491727 CAPLUS

DOCUMENT NUMBER: 71:91727

ORIGINAL REFERENCE NO.: 71:17095a,17098a

TITLE: Mass spectrometric fragmentation in the Cinchona alkaloid series

AUTHOR(S): Begue, Jean P.; Fetizon, Marcel

CORPORATE SOURCE: Lab. Stereochim., Fac. Sci., Orsay, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1969), (4), 1251-4

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

GI For diagram(s), see printed CA Issue.

AB Major cleavage of quinine in mass spectrometry yields fragments in which H is transferred from quinuclidine to quinoline moieties. In expts. with I-2-d and II-2- and -3-d, the 2-H (D) was transferred to the aryl fragment during mass spectral cleavage. Condensing aromatic aldehydes and 3-quinuclidone with NaOEt in EtOH gave III (R, m.p., and % yield listed): 4-quinolyl, 154-5°, 60; Ph, 133°, 85; 4-pyridyl, 140°, 46; 1-naphthyl, 149°, 75. Hydrogenation of III over Pd gave I (R, m.p., and % yield listed): 4-quinolyl, 126-7°, 55; Ph, 84-5°, 67; 4-pyridyl, 114-16°, 70; 1-naphthyl, 97-8°, 72. I with NaBH₄ yielded II (R, m.p., and % yield listed): 4-quinolyl, 215°, 52; (prepared by hydrogenation over Pt), 156-7°, -; 4-pyridyl, 129-30°, 60; 1-naphthyl, 169.5-70° and 211-13.5° (stereoisomers), -. I with D₂O and K₂CO₃ gave I-2-d, which were reduced with LiAlH₄ to II-2-d. I with LiAlD₄ gave II-3-d.

IT 24177-70-6P 24177-72-8P 24177-73-9P

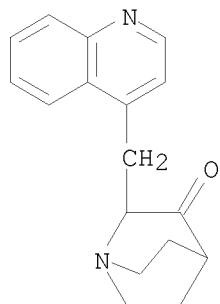
24177-77-3P 24177-78-4P 24177-79-5P

24177-80-8P 28281-22-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

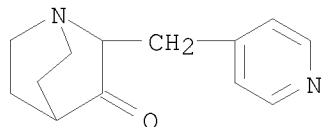
RN 24177-70-6 CAPLUS

CN 11-Norcinchonane-7-one, (8ξ)- (9CI) (CA INDEX NAME)

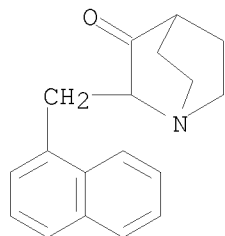


RN 24177-72-8 CAPLUS

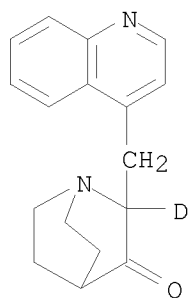
CN 3-Quinuclidinone, 2-(4-pyridylmethyl)- (8CI) (CA INDEX NAME)



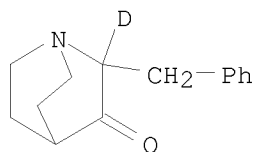
RN 24177-73-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(1-naphthalenylmethyl)- (CA INDEX NAME)



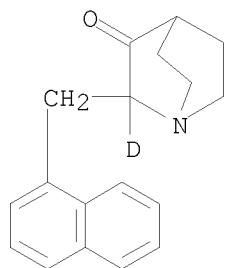
RN 24177-77-3 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(4-quinolylmethyl)- (8CI) (CA INDEX NAME)



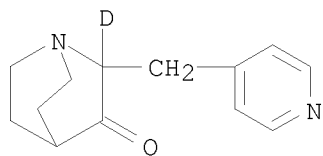
RN 24177-78-4 CAPLUS
CN 3-Quinuclidinone-2-d, 2-benzyl- (8CI) (CA INDEX NAME)



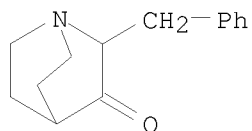
RN 24177-79-5 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(1-naphthylmethyl)- (8CI) (CA INDEX NAME)



RN 24177-80-8 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(4-pyridylmethyl)- (8CI) (CA INDEX NAME)



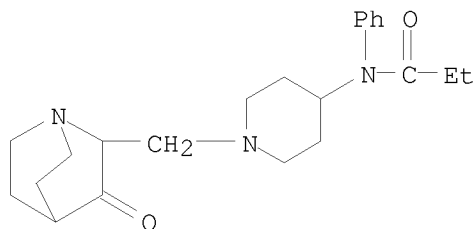
RN 28281-22-3 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(phenylmethyl)- (CA INDEX NAME)



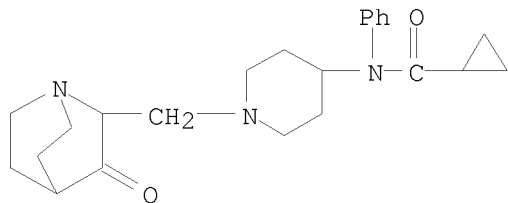
L15 ANSWER 123 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1969:491343 CAPLUS
 DOCUMENT NUMBER: 71:91343
 ORIGINAL REFERENCE NO.: 71:17003a,17006a
 TITLE: 2-(4-Anilinopiperidinomethyl)-3-quinuclidinones
 exhibiting antidepressant activity
 INVENTOR(S): Biel, John H.; Hopps, Harvey B.
 PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3462442	A	19690819	US 1965-515183	19651220 <--
PRIORITY APPLN. INFO.:			US 1965-515183	A 19651220

GI For diagram(s), see printed CA Issue.
 AB Title compds. with the described activity are prepared Thus, 50 g.
 3-quinuclidinone, 50 g. 37% aqueous HCHO, and 68 g. 40% aqueous Me₂NH in 70 ml.
 absolute EtOH is refluxed 22 hrs. to give 43 g. 2-methylene-3-quinuclidinone
 (I), b₁₀ 90-110°. A solution of 5.48 g. I and 9.28 g.
 4-(N-propionylanilino)piperidine in 100 ml. MeOH is kept 24 hrs. to give
 II, m. 123-4°. Similarly prepared is III, m. 129-31°.
 IT 23851-86-7P 23851-87-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 23851-86-7 CAPLUS
 CN Propionanilide, N-[1-[(3-oxo-2-quinuclidinyl)methyl]-4-piperidyl]- (8CI)
 (CA INDEX NAME)



RN 23851-87-8 CAPLUS
 CN Cyclopropanecarboxanilide, N-[1-[(3-oxo-2-quinuclidinyl)methyl]-4-
 piperidyl]- (8CI) (CA INDEX NAME)



L15 ANSWER 124 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:430341 CAPLUS

DOCUMENT NUMBER: 71:30341

ORIGINAL REFERENCE NO.: 71:5589a,5592a

TITLE: Antimalarials. Some quinuclidine derivatives of
7-chloro-4-aminoquinoline and 6-methoxy-8-
aminoquinoline

AUTHOR(S): Singh, Tara; Stein, Robert G.; Koelling, Harlan H.;
Hoops, John F.; Biel, John H.

CORPORATE SOURCE: Res. Lab., Aldrich Chem. Co., Inc., Milwaukee, WI, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12,
524-6

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Thirteen quinoline compds. containing quinuclidine rings in side chains were
prepared and tested for their antimalarial activity against Plasmodium
berghei in mice. 7-Chloro-4-(3-oxoquinuclidinyl)-2-
methyleneamino)quinoline (I) and 7-chloro-4-(3-hydroxyquinuclidinyl)-2-
methyleneamino)quinoline (II) were curative; I cured 2 mice at 160 mg./kg.
and all 5 in the test at 640 mg./kg., while II showed slight activity at
160 and 320 mg./kg. and cured all 5 mice at 640 mg./kg. All other compds.
were inactive and toxic.

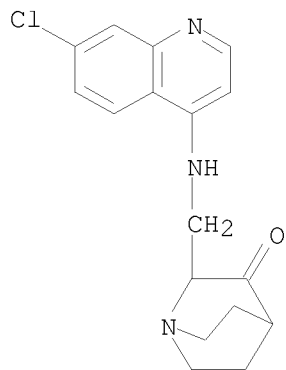
IT 21566-68-7P 22776-50-7P 22776-52-9P

22950-03-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

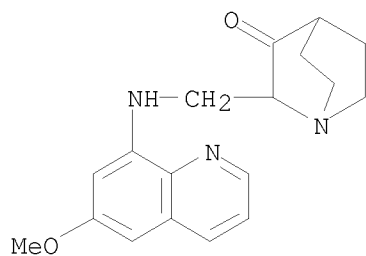
RN 21566-68-7 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[(7-chloro-4-quinolinyl)amino]methyl]-
(CA INDEX NAME)

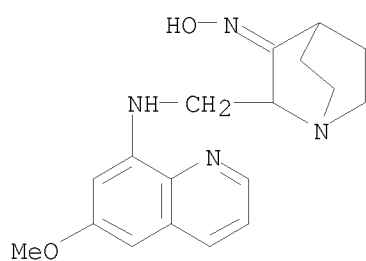


RN 22776-50-7 CAPLUS

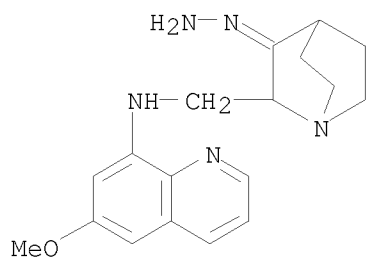
CN 3-Quinuclidinone, 2-[[[(6-methoxy-8-quinolyl)amino]methyl]- (8CI) (CA
INDEX NAME)



RN 22776-52-9 CAPLUS
 CN 3-Quinuclidinone, 2-[[6-methoxy-8-quinolyl]amino]methyl]-, oxime (8CI)
 (CA INDEX NAME)



RN 22950-03-4 CAPLUS
 CN 3-Quinuclidinone, 2-[[6-methoxy-8-quinolyl]amino]methyl]-, hydrazone
 (8CI) (CA INDEX NAME)



L15 ANSWER 125 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:459119 CAPLUS
DOCUMENT NUMBER: 69:59119
ORIGINAL REFERENCE NO.: 69:11047a,11050a
TITLE: 2-Methylene-3-quinuclidinone
INVENTOR(S): Biel, John H.; Hopps, Harvey B.; Bader, Henryk
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3384641	A	19680521	US 1967-668941	19670919 <--
PRIORITY APPLN. INFO.:			US 1967-668941	A 19670919

GI For diagram(s), see printed CA Issue.

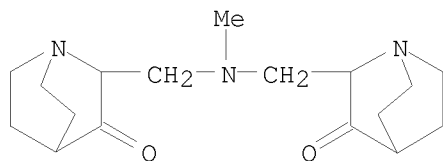
AB The title compound (I) is prepared by heating the Mannich reaction product of 3-quinuclidinone (II), Me₂NH, and HCHO; it is used to sep. tertiary from primary and secondary amines. Thus, 200 g. II, 270 g. 40% Me₂NH, 194.8 g. 37% HCHO, 250 ml. EtOH, and 100 ml. water was refluxed 1 hr., held 17 hrs. at 70°, and worked up to give 203 g. I, b₇ 91-2°, n_D 1.5110; HCl salt m. 284-8°. A mixture of pyridine and piperidine was separated by distillation in the presence of I. The piperidine distilled only after its reaction product with I decomposed. MeNH₂ was also purified by adding 13.7 g. I in 20 ml. MeOH to 3.88 g. 40% aqueous MeNH₂ and heating 1 hr. at 50° to give 11 g. 2,α'-methyliminobis(2-methyl-3-quinuclidinone) monohydrate, m. 90-2°, which was decomposed by gentle heating to pure MeNH₂, leaving I as a residue.

IT 19576-25-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19576-25-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis-
(9CI) (CA INDEX NAME)



L15 ANSWER 126 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:427579 CAPLUS
DOCUMENT NUMBER: 69:27579
ORIGINAL REFERENCE NO.: 69:5155a,5158a
TITLE: Synthetic quinine analogs. I. Synthesis and some chemical transformations of 6'-methoxy-7-oxo-8-rubene
AUTHOR(S): Bender, D. R.; Coffen, D. L.
CORPORATE SOURCE: Univ. of Colorado, Boulder, CO, USA
SOURCE: Journal of Organic Chemistry (1968), 33(6), 2504-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

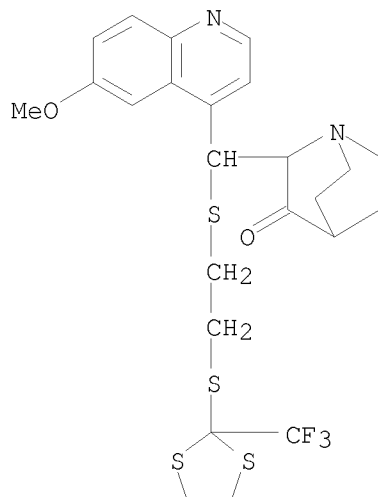
AB NaOEt-catalyzed condensation of 6-methoxyquinoline-4-carboxaldehyde with 3-quinuclidinone produces 6'-methoxy-7-oxo-8-rubene (I) in high yield. Of the 2 possible geometrical isomers, only that with the ketone function trans to the quinoline ring is formed. Reduction of I affords an allylic alc. whose p-nitrobenzoate is completely isomerized to the opposite geometrical isomer in refluxing HOAc. I is not ketalized by 1,2-ethanedithiol in refluxing F3CCO2H involving 1 mol. of ketone, 2 of 1,2-ethanedithiol, and 1 of F3CCO2H. A by-product of the reaction results from the condensation of 3 mols. of 1,2-ethanedithiol with 2 of F3CCO2H. Pyrazoline derivs. of I resulting from 1,3-dipolar addition of CH2N2 and condensation with hydrazine are described. 24 references.

IT 16526-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16526-37-7 CAPLUS

CN Orthoacetic acid, trifluorotrithio-, cyclic ethylene ester, ester with 2-[[[(2-mercaptoethyl)thio](6-methoxy-4-quinolyl)methyl]-3-quinuclidinone, (±)- (8CI) (CA INDEX NAME)



L15 ANSWER 127 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1966:84473 CAPLUS

DOCUMENT NUMBER: 64:84473

ORIGINAL REFERENCE NO.: 64:15837a-b

TITLE: Systems with bridgehead nitrogen. β -Ketols of the 1-azabicyclo[2.2.2]octane series

AUTHOR(S): Nielsen, Arnold T.

CORPORATE SOURCE: Chem. Div., U.S. Naval Ordnance Test Sta., China Lake, CA

SOURCE: Journal of Organic Chemistry (1966), 31(4), 1053-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

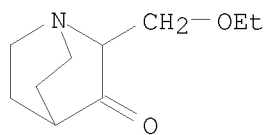
AB The preps. and chemical behavior of the β -ketols incorporating the 1-azabicyclo [2.2.2] octane ring are described. Three different structural types are represented in this study. Methylation of 3-quinuclidinone with excess formaldehyde (potassium carbonate catalyst under appropriate conditions) led to 2,2-bismethylol-3-quinuclidinone (I) or 2-methylene-3-quinuclidinone (II). 2-Methylol-3-quinuclidinone (III) was prepared by hydration of II cation. Starting with 4-acetylpiperidine and its N-benzyl derivative, syntheses of 4-hydroxymethyl-3-quinuclidinone (IV) and 4-acetyl-3-quinuclidinol (V) were achieved. The bridgehead IV was extremely stable whereas V underwent facile retrograde aldolization in basic media. I readily loses one methylol group in base leading to III, which dehydrates with extreme ease rather than undergo demethylation.

IT 5291-13-4P, 3-Quinuclidinone, 2-(ethoxymethyl)- 5291-14-5P, 3-Quinuclidinone, 2-methyl- 5291-27-0P, 3-Quinuclidinone, 2-(hydroxymethyl)- 5291-32-7P, 3-Quinuclidinone, 2-(hydroxymethyl)-2-(methoxymethyl)- 5291-33-8P, 3-Quinuclidinone, 2-(ethoxymethyl)-, picrate 5291-34-9P, 3-Quinuclidinone, 2-methyl-, picrate 5291-35-0P, 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride

RL: PREP (Preparation)
(preparation of)

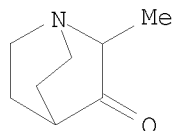
RN 5291-13-4 CAPLUS

CN 3-Quinuclidinone, 2-(ethoxymethyl)- (7CI, 8CI) (CA INDEX NAME)



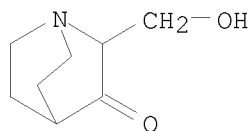
RN 5291-14-5 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)

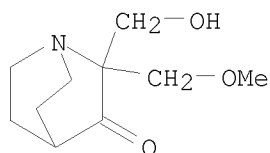


RN 5291-27-0 CAPLUS

CN 3-Quinuclidinone, 2-(hydroxymethyl)- (7CI, 8CI) (CA INDEX NAME)



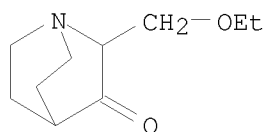
RN 5291-32-7 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)- (CA INDEX NAME)



RN 5291-33-8 CAPLUS
 CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(ethoxymethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

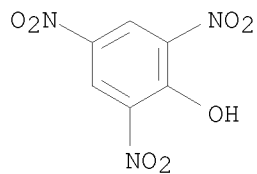
CM 1

CRN 5291-13-4
 CMF C10 H17 N O2



CM 2

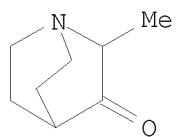
CRN 88-89-1
 CMF C6 H3 N3 O7



RN 5291-34-9 CAPLUS
 CN 3-Quinuclidinone, 2-methyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

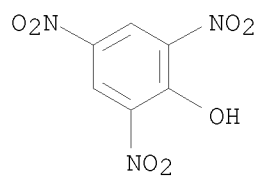
CRN 5291-14-5
 CMF C8 H13 N O



CM 2

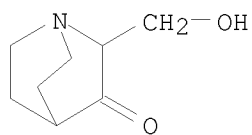
CRN 88-89-1

CMF C6 H3 N3 O7



RN 5291-35-0 CAPLUS

CN 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

ACCESSION NUMBER: 1964:9663 CAPLUS
 DOCUMENT NUMBER: 60:9663
 ORIGINAL REFERENCE NO.: 60:1697e-h,1698a-h,1699a
 TITLE: Quinuclidine series. VII. Solvolysis of
 2-(α -chlorobenzyl)quinuclidine. The
 heterocinchonine rearrangement
 AUTHOR(S): Braschler, V.; Grob, C. A.; Kaiser, A.
 CORPORATE SOURCE: Univ. Basel, Switz.
 SOURCE: Helvetica Chimica Acta (1963), 46(7),
 2646-58
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 60:9663

AB cf. CA 53, 4278e. The rate and the products of the hydrolysis of
 2-(α -chlorobenzyl)quinuclidine (I) do not provide evidence for the
 participation of the quinuclidine N in the ionization step, and no product
 derived from a heterocinchonine rearrangement could be isolated.
 2-Benzyl-2-dehydroquinuclidine (II) and 2-benzylidenequinuclidine (III)
 possess abnormal spectral and chemical properties ascribable to steric
 inhibition of the vinylamine-type mesomerism. Et isonicotinate (151 g.)
 and 167 g. BrCH₂CO₂Et in 500 cc. EtOH kept at room temperature overnight,
 refluxed 4 hrs., hydrogenated 0.5-1 hr. at 90°/100 atmospheric over 15 g.
 10% Pd-C, filtered, the filtrate evaporated at 50-60°, the semicryst.
 residue treated with cooling and shaking with 500 cc. cold H₂O, 500 cc.
 CHCl₃, and 150 g. K₂CO₃ in 250 cc. H₂O, and the organic layer worked up
 yielded 180-90° 4-carbethoxy-1-carbethoxymethylpiperidine (IV),
 b_{0.2} 111-13°, n_{20D} 1.4585, d₁₅₁₅ 1.057. IV (100 g.) in 250 cc.
 absolute MePh added dropwise during 1.5 hrs. to KOEt (from 39.096 g. K and 60
 cc. EtOH in 162 cc. dry MePh) the mixture stirred 4 hrs. at 130°,
 cooled, the MePh decanted, extracted with 50 cc. H₂O, the residue dissolved in
 300 cc. EtOH, combined with the aqueous extract, the solution adjusted with
 100 cc.
 10N HCl with cooling and stirring to pH 7 below 30°, cooled to
 0°, filtered, the filtrate adjusted with about 2 cc. AcOH to pH 4,
 concentrated to about 200 cc., treated with 20 cc. saturated aqueous KHCO₃,
 and extracted
 with CHCl₃ yielded 57 g. 2-carbethoxy-3-quinuclidone (V), b_{0.02}
 98-103°, m. 116-20° (absolute EtOH-Et₂O). V (20 g.), 80 cc. dry
 Et₃N, and 100 cc. absolute EtOH hydrogenated over about 5 g. Raney Ni under
 ambient conditions yielded 10.9 g. 2-carbethoxy-3-hydroxyquinuclidine (VI)
 isomer A (VII), m. 147-8° (Me₂CO), (sublimation); the filtrate was
 evaporated and the cryst, residue (9 g.) chromatographed on 200 g. Al₂O₃ to
 give 2.34 g. VII, 4.7 g. isomer mixture, m. 72-105°, and 1.98 g. VI
 isomer B, m. 100-2°; VI.MeI, m. 175-8° (decomposition)
 (EtOH-Et₂O). VI (21.1 g.) and 150 cc. Ac₂O refluxed 6 hrs., the mixture
 evaporated, the oily residue partitioned between 200 cc. Et₂O and 50 cc. 2N
 HCl, the Et₂O phase extracted with 2N HCl, the combined aqueous solns.
 saturated with
 solid K₂CO₃, and extracted with Et₂O gave 14.4 g. 2-carbethoxy-2-
 dehydroquinuclidine (VIII), b₁₂ 128-30°, n_{25D} 1.4955, and 1.1 g.
 acetate of VI, b₁₂ 130-63°. VIII (12.7 g.) in 65 cc. EtOH
 hydrogenated 1 hr. over 600 mg. 10% Pd-C under ambient conditions yielded
 12.1 g. 2-carbethoxyquinuclidine, b₁₁ 119-20°, n_{25D} 1.4752, b₁₁
 119-20°; picrate m. 120° (EtOH). VIII (10 g.) and 150 cc.
 saturated NH₃-MeOH heated 15 hrs. at 100° in an autoclave gave 7.5 g.
 2-CONH₂ analog (IX) of VIII, m. 178-81° (Me₂CO). IX (5.45 g.) in
 50 cc. MeOH and 25 cc. H₂O hydrogenated 2 hrs. over Raney Ni W-7 under
 ambient conditions yielded 4.9 g. 2-carbamoylquinuclidine (X), m.
 148-9° (Me₂CO). 2-Carbethoxyquinuclidine (1.2 g.) and 10 cc.
 NH₃-MeOH (saturated at 20°) heated 48 hrs. at 100° in a sealed

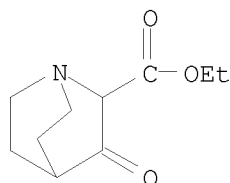
tube gave 0.81 g. X, m. 145-6° (Me₂CO). IX (5.6 g.) in 45 cc. Et₃N and 25 cc. CHCl₃ mixed with 10.5 g. P₂O₅ and 50 g. sand, refluxed 30 hrs., cooled, the supernate decanted, the residual oil washed with Et₂O, the residue treated with saturated aqueous K₂CO₃ and extracted with Et₂O, and the combined washings, and decantate worked up yielded 0.92 g. unreacted IX, m. 177-80°; the mother liquor distilled gave 2 g. 2-CN analog of VIII, b₁₁ 120-3°, n_D²⁰ 1.5068. X (12.2 g.), 22.5 g. P₂O₅, and 50 g. sand refluxed 26 hrs. with 90 cc. dry Et₃N and 60 cc. dry CHCl₃ and similarly worked up yielded 8.25 g. 2-cyanoquinuclidine (XI), b₁₃ 105-21°; picrate m. 216-26° (decomposition) (Me₂CO-EtOH); XI.MeI m. 247-50° (decomposition) (absolute EtOH). X (9.4 g.), 50 cc. Ac₂O, and 50 cc. Et₃N refluxed 10 hrs. yielded 4 g. XI, b₁₃ 105-21°. XI (17.4 g.) in 300 cc. dry C₆H₆ added dropwise during 1 hr. to PhMgBr from 6.5 g. Mg, 40.2 g. PhBr, and 170 cc. dry Et₂O and the mixture refluxed 4 hrs. yielded 20.9 g. 2-benzoylquinuclidine (XII), m. 88-9.5° (Et₂O); the residue from the mother liquor sublimed at 120-40°/11 mm. gave 1.35 g. XII, m. 86-9°; picrate m. 174-8° (EtOH); methiodide m. 196-8° (Me₂CO). XII (1 g.) and 0.335 g. NH₂OH.HCl in 20 cc. MeOH refluxed 24 hrs. yielded the oxime of XII, m. 194-5.5° with sublimation (AcOEt); picrate m. 194-8° with sublimation (EtOH) XII (4.0 g.) in 50 cc. dry Et₂O added dropwise during 10 min. with stirring to 0.5 g. LiAlH₄ in 50 cc. dry Et₂O, the mixture refluxed 3 hrs., stirred 12 hrs. at room temperature, and decomposed with 30 cc. iced H₂O and 25 cc. concentrated HCl yielded the mixed isomeric 2-(α-hydroxybenzyl)quinuclidine (XIII), which-recrystd. repeatedly from Me₂CO gave 800 mg. isomer A (XIIIa), m. 142-4° [picrate m. 191-4° (EtOH)]; the residue (2.9 g.) from the mother liquor chromatographed on 60 g. Al₂O₃ gave the isomer B (XIIIb), m. 75-6.5° (petr. ether) [picrate m. 183-6° (EtOH)]. XIII (3 g.) and 30 cc. SOCl₂ refluxed 12 hrs., the mixture evaporated, and the residue evaporated twice with C₆H₆ and fractionally recrystd. from absolute EtOH yielded I.HCl isomer A (Ia.HCl), m. 238-40° (absolute EtOH-Et₂O) [picrate m. 183-6° (EtOH)], and I.HCl isomer B (Ib.HCl), m. 245-9.5° (decomposition) [picrate m. 173-4° (EtOH)]. Ia (1.89 g.) in 5 cc. absolute EtOH refluxed 3 hrs. with 3.5 g. KOH in 20 cc. absolute EtOH yielded 1.39 g. III isomer A (IIIa), b₁₂ 168-70° [picrate m. 149-50° and then 167-9° (EtOH)]. Ib (500 mg.) and 1 g. KOH in 10 cc. absolute EtOH refluxed 14 hrs. yielded 394 mg. oily III isomer B (IIIb) [picrate m. 162-3° and then 180-1° (iso-PrOH-Me₂CO)]. Quinuclidone-HCl (8.5 g.) and 15 g. BzH refluxed 10 hrs. with 7.5 g. KOH in 150 cc. absolute EtOH yielded 8.07 g. 2-benzylidene-3-quinuclidone (XIV), m. 134-7° (MeOH) [picrate m. 180-4° (EtOH)]. XIV (11.05 g.) in 300 cc. MeOH hydrogenated under ambient conditions over Raney Ni, and the product fractionally recrystd. from Me₂COMeOH yielded 7.7 g. 2-benzyl-3-hydroxyquinuclidine isomer A (XVa), m. 157-8° [picrate m. 128-32° (iso-PrOH); HCl salt m. 203-7° (MeOH-Me₂CO-Et₂O)]; the residue (2.85 g.) from the mother liquor chromatographed on 60 g. Al₂O₃ yielded 1.5 g. XV isomer B (XVb), m. 129-33° (Me₂CO) [picrate, m. 159-62° (iso-PrOH)], and 1.3 g. mixed XVa and XVb. XVa (5 g.) and 50 cc. SOCl₂ refluxed 70 hrs. gave 2 g. II, b₀ 0.005 62°, n_D²³ 1.5485, which solidified at -15° [picrate m. 200-5° (Me₂CO)], and 1.9 g. 2-benzyl-3-chloroquinuclidine, b₀ 0.005 73-5°, picrate m. 184-7° with a change to plates and then m. 201-3° (iso-PrOH). I.HCl (500 mg.) in 25 cc. EtOH hydrogenated about 2 hrs. over 50 mg. 10% Pd-C yielded 2-benzylquinuclidine-HCl (XVI.HCl), m. 268-9° (EtOH-Et₂O) (with sublimation); picrate m. 184-6° (EtOH). IIIa or IIIb (200 mg.) in EtOH hydrogenated over Pd-C yielded XVI isolated as picrate, m. 183-6° (EtOH); XVI.HCl m. 270-2° (EtOH-Et₂O). II (260 mg.) in 5 cc. EtOH hydrogenated over Raney Ni yielded XVI isolated as the picrate, m. 180.5-3.5° (iso-PrOH). I.HCl (2.0017 g.), 8 cc. N NaOH, 32.4 cc. H₂O, and 32.4 cc. Me₂CO heated 24 hrs. at 68°,

cooled, acidified with 2N HCl, concentrated to 20 cc. at 45°, basified with saturated aqueous K₂CO₃, and extracted with CHCl₃, and the residue from the extract chromatographed on Al₂O₃ yielded 100 mg. substance which gave the picrate of IIIa, m. 145-50° and then 167-9° (EtOH), 110 mg. oil which yielded the picrate of XIII, m. 278-81° (EtOH) [free base m. 72-8° (petr. ether)], and 110 mg. oily C₁₃H₁₇NO (XVII); picrate m. 186-8° (EtOH); HCl salt m. 157-8° (decomposition) (iso-PrOH-Et₂O). I.HCl (4 g.), 5.94 g. Et₃N, 40 cc. H₂O, and 40 cc. Me₂CO refluxed 42 hrs., cooled, acidified with 2N HCl, concentrated to 30 cc., basified with saturated aqueous K₂CO₃, and extracted with Et₂O, and the oily residue (3.1 g.) from the extract chromatographed on Al₂O₃ gave 103 mg. III, 210 mg. XIII, and 56 mg. XVII. I.HCl (1.3 g.) treated in the usual manner with K₂CO₃, the free base stirred 24 hrs. at room temperature in 100 cc. 60% aqueous Me₂CO with 2 equivs. Ag₂O, refluxed 24 hrs., filtered through Celite, acidified with 2N HCl, concentrated to 20 cc., basified with saturated aqueous K₂CO₃, and extracted with CHCl₃, and the oily residue from the extract distilled gave 510 mg. yellow oil, b_{0.01} 90-110°, which chromatographed on Al₂O₃ yielded 147 mg. III, 89 mg. XIII, and 155 mg. oily XVII.

IT 34286-16-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester
 RL: PREP (Preparation)
 (preparation of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



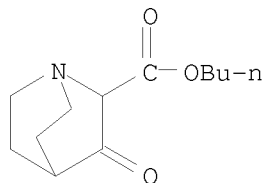
L15 ANSWER 129 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:410798 CAPLUS
DOCUMENT NUMBER: 57:10798
ORIGINAL REFERENCE NO.: 57:2192e-i
TITLE: Synthesis of 2,3-quinuclidinedicarboxylic acid
AUTHOR(S): Mikhлина, E. E.; Rubtsov, M. V.; Vorob'eva, V. Ya.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem.-Pharm. Res. Inst.,
Moscow
SOURCE: Zhurnal Obshchei Khimii (1961), 31, 3251-5
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10798

AB cf. CA 54, 9945i. Azeotropic removal of H₂O from 69.3 g. KOH, 11. BuOH, and 100 ml. MePh, evaporation of the residue, and treatment with 120 g. 1-carbethoxymethyl-4-carbethoxypiperidine 5 hr. in MePh gave a viscous mass containing K salt of the enol of Bu 3-oxoquinuclidine-2-carboxylate, which treated with 10% AcOH followed by K₂CO₃ gave 43.5% Bu 3-oxo-quinuclidine-2-carboxylate, b_{0.6} 137° m. 88°; HCl salt m. 163°. The latter treated with aqueous KCN at 5° gave 68.5% cyanohydrin, m. 107°. Similarly was prepared the cyanohydrin of the Et ester, m. 124-5°. This refluxed 25 hrs. with AcOH-HCl then esterified with EtOH-HCl gave some 3-quinuclidone, separated by sublimation, and 30% di-Et 3-hydroxyquinuclidine-2,3-dicarboxylate (I), b_{1.2} 142°, m. 104-5°, also formed from the corresponding Bu ester cyanohydrin. Refluxing the di-Et ester with 1:1 HCl 5 hrs. gave 65% 3-hydroxyquinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 126°. I with SOCl₂ 30 hrs. followed by aqueous K₂CO₃ gave 74.5% di-Et Δ²-dehydroquinuclidine-2,3-dicarboxylate, b_{0.5} 130°; HCl salt m. 148.5°. This refluxed 5 hrs. with 1:1 HCl gave 99% Δ²-dehydroquinuclidine-2,3-dicarboxylic acid, decomposed at 240°; HCl salt, hygroscopic crystals, hydrolyzed by H₂O. Hydrogenation over Pt gave quinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 138°, which refluxed 5 hrs. with EtOH-HCl gave the di-Et ester (II), b_{0.4} 115°, which with LiAlH₄ gave 58% 2,3-bis(hydroxymethyl)quinuclidine, b_{0.3} 150°; HCl salt, hygroscopic crystals. This and AcCl in refluxing CHCl₃ 5 hrs. gave 70% diacetate, b_{0.6} 138-40°. II kept 7 days in H₂O gave 83.5% 3-carbethoxyquinuclidine-2-carboxylic acid, decomposed at 188-9°.

IT 91554-81-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride 91554-82-4P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester
RL: PREP (Preparation)
(preparation of)

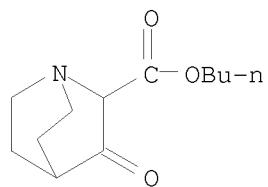
RN 91554-81-3 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride (7CI)
(CA INDEX NAME)



● HCl

RN 91554-82-4 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester (7CI) (CA INDEX NAME)



L15 ANSWER 130 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

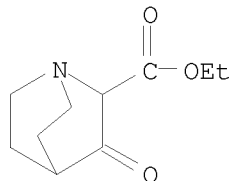
ACCESSION NUMBER: 1960:50470 CAPLUS
DOCUMENT NUMBER: 54:50470
ORIGINAL REFERENCE NO.: 54:9945i,9946a-c
TITLE: Amino acids of the quinuclidine series
AUTHOR(S): Yakhontov, L. N.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Research
Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 2343-8
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:50470

AB Keeping 1.1 g. 2-formylquinuclidine and 0.9 g. EtO₂CCH₂CN in 3 ml. pyridine with 5 drops piperidine 10 days gave a precipitate of 97.2% Et β -(2-quinuclidyl)- α -cyano-acrylate, m. 139.5-41° (picrate, m. 130.5-10°), which hydrogenated over Pt to α -aminomethyl- β -(2-quinuclidyl)propionic acid, isolated as dipicrate, decomposing 125°; the acid was isolated after the original reaction mixture was hydrogenated and then refluxed with concentrated HCl. Keeping an aqueous solution of Na salt of enol form of Et β -(2-quinuclidyl)- β -oxopropionate 1 day gave Na β -(2-quinuclidyl)- β -oxopropionate, decomposing 240°; this with HONH₂ gave 93% β -(2-quinuclidyl)- β -oxopropionic acid oxime, an oil; di-HCl salt, decompose 284°; picrate, m. 167-70°. Hydrogenation of the oxime over Pt gave 78% β -(2-quinuclidyl)- β -aminopropionic acid isolated as di-HCl salt, decomposing 283°. To KOEt in dry MePh was added at 120° 1-carbethoxymethylisonipecotinic acid, the whole was refluxed 5 hrs., cooled, the precipitated K salt of Et 3-oxo-2-quinuclidinecarboxylate was separated and treated with dilute AcOH, yielding

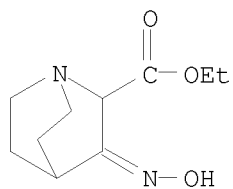
75%

Et 3-oxo-2-quinuclidinecarboxylate, m. 109-10°. This with HONH₂.HCl in EtOH gave 80% corresponding oxime, isolated as HCl salt, decomposing 196°. This, hydrogenated over Pt to 99.4% Et 3-amino-2-quinuclidinecarboxylate di-HCl salt, decomposing 185°. This heated with concentrated HCl 6 hrs. gave 91% 3-amino 2-quinuclidinecarboxylic acid di-HCl salt, decomposing 242°.

IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

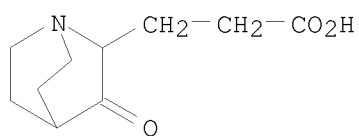


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)

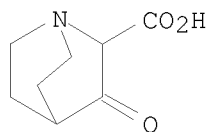


● HCl

RN 117342-57-1 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 857019-15-9, 2-Quinuclidinecarboxylic acid, 3-oxo-
 (derivs.)
 RN 857019-15-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo- (CA INDEX NAME)



ACCESSION NUMBER: 1960:50469 CAPLUS
DOCUMENT NUMBER: 54:50469
ORIGINAL REFERENCE NO.: 54:9945d-i
TITLE: Phenanthryl substituted barbiturates
AUTHOR(S): Giannini, M.; Fedi, M.; Russo, F.
CORPORATE SOURCE: Lab. chim. farm. A. Menarini, Florence
SOURCE: Bollettino Chimico Farmaceutico (1959), 98,
714-21
CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Refluxing 2.26 g. 9-(chloromethyl)phenanthrene (I) with 62 ml. PrOH, adding 1.42 g. 5-methylbarbituric acid and 0.8 g. HCO₂Na in 7 ml. H₂O, refluxing 7 hrs., distilling the PrOH to a small volume, mixing the residue with

100 ml. H₂O, filtering, and washing with C₆H₆ until the product was colorless, gave 0.8 g. 5-(9-phenanthrylmethyl)-5-methylbarbituric acid, m. 233-5° (MePh). Refluxing 2.26 g. I in 62 ml. PrOH with 1.56 g. ethylbarbituric acid and 0.8 g. AcONa in 7 ml. H₂O for 5 hrs., distilling the solvent, taking up with 100 ml. H₂O, allowing to stand, and washing with C₆H₆ gave 1.2 g. 5-(9-phenanthrylmethyl)-5-ethylbarbituric acid (II), m. 237-8° (xylene). By an analogous procedure there were prepared the following analogs of II: 5-Pr, m. 240° (MePh); 5-Bu, m. 245-8° (MePh and C₆H₆); 5-allyl, m. 228-30° (xylene). Adding to 6.3 g. K₂Cr₂O₇ in 19 g. H₂SO₄ and 31 ml. H₂O at water bath

temperature

2 g. I, adding later 6.3 g. K₂Cr₂O₇, heating to boiling, cooling, diluting with H₂O, washing thoroughly, digesting the solid with NaHSO₃ solution at 50-60°, precipitating the phenanthrenequinone with dilute H₂SO₄ and subliming gave the pure quinone, m. 204°. Treating this quinone in EtOH with o-phenylenediamine gave the corresponding phenazine, m. 217°.

Refluxing 2 g. II 48 hrs. with 20 ml. 25% NaOH solution and 20 ml. EtOH, diluting with H₂O, acidifying with 10% H₂SO₄, keeping for crystallization, filtering,

dissolving with NaHCO₃ solution, precipitating with H₂SO₄, dissolving in Et₂O, and

precipitating with petr. ether gave 0.5 g. ethyl-(9-phenanthrylmethyl)malonic acid, m. 152-4° (decomposition). Refluxing 2.26 g. I with 1.58 g. 5-methyl-2-thiobarbituric acid in 60 ml. PrOH to dissoln., adding 0.8 g. NaOAc in 7 ml. H₂O, refluxing 1 hr., distilling the PrOH to a small volume, adding 100 ml. H₂O, washing the crystals with C₆H₆, dissolving repeatedly in NaOH and precipitating with HCl gave 2.15 g.

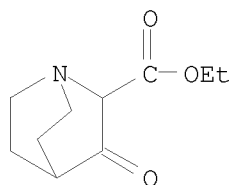
5-(9-phenanthrylmethyl)-5-methyl-2-thiobarbituric acid, m. 280-2°. By an analogous procedure with 0.1 mole material were prepared 3.4 g. 5-Et analog., 250-3° (xylene), 2.5 g. Pr analog. m. 230-1° (xylene), 0.8 g. Bu analog, m. 210° (xylene), and 0.8 g. allyl analog m. 185-9° (MePh). Dissolving 7.4 g. Na in 135 anhydrous EtOH, adding 8.5 g. thiourea and 20 g. di-Et allylmalonate, refluxing 4 hrs., dissolving the precipitate in a min. volume of H₂O, and precipitating with HCl gave 3.52 g. 5-allyl-2-thiobarbituric acid, m. 120-2° (xylene). By the same method was prepared from 11.5 g. thiourea and 25 g. di-Et propylmalonate 5.37 g. 5-propyl-2-thiobarbituric acid, m. 163-5° (H₂O).

IT 34286-16-3 110056-51-4 117342-57-1

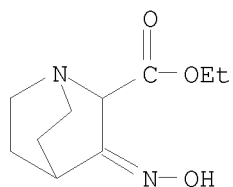
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

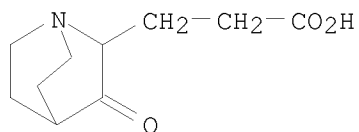


RN 110056-51-4 CAPLUS
 CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride
 (6CI) (CA INDEX NAME)



● HCl

RN 117342-57-1 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)

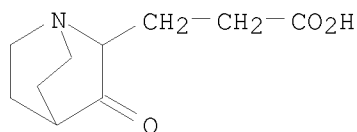


ACCESSION NUMBER: 1959:122172 CAPLUS
 DOCUMENT NUMBER: 53:122172
 ORIGINAL REFERENCE NO.: 53:21953f-i,21954a-c
 TITLE: Cyanoethylation of 3-quinuclidinone
 AUTHOR(S): Mikhлина, E. E.; Rubtsov, M. V.
 CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research
 Inst., Moscow
 SOURCE: Zhurnal Obshchei Khimii (1959), 29, 118-24
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Na (24 g.) in 100 ml. MePh and 36 ml. absolute EtOH heated to 120-5°, treated over 1 hr. with 60 g. 1-carbethoxymethyl-4-carbethoxypiperidine in 150 ml. MePh, refluxed 5 hrs., treated with 200 ml. concentrated HCl, the mixture stirred 0.5 hr., the organic layer separated, reextd. with 200 ml. concentrated HCl twice, the acid exts. combined, refluxed 15 hrs., decolorized, and the residue evaporated, treated with 50% KOH, and extracted with C₆H₆ gave 84.6% 3-quinuclidinone, m. 136-8°; picrate, m. 210°. This (25 g.) in 115 ml. dry dioxane and 3.8 ml. 30% KOH in MeOH heated to 60°, treated over 0.5 hr. with 90 ml. CH₂:CHCN, stirred 4 hrs. at 60°, the amorphous polymer filtered off, the filtrate freed of dioxane in vacuo, the residue treated with 100 ml. C₆H₆, extracted with 50 ml. 10% HCl, and the acid extract treated with K₂CO₃, and extracted with C₆H₆ yielded on distillation 14.3 g. 3-quinuclidinone. The distillation residue with 20 ml. absolute EtOH and 1 ml. dry C₆H₆ yielded 4 g. 3-oxo-2,2-bis(2-cyanoethyl)quinuclidine (Ia), m. 120-2° (EtOH); the mother liquor gave 0.7 g. 3-oxo-2-(2-cyanoethyl)quinuclidine (I), b_{0.3} 121-2°. The same products were formed in Me₃COH with MeOH-KOH catalyst. Refluxing I with HCl-AcOH 20 hrs. gave crude 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, which, heated 3 hrs. with 9% alc.-dry HCl gave 60.6% 3-oxo-2-(2-carbethoxyethyl)quinuclidine (II), b_{0.4} 136-8°, after the usual treatment of the mixture with K₂CO₃; the ester refluxed 4 hrs. with 17% HCl gave 96.5% 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, decompose 191-3° (EtOH). Heating 0.3 g. II and 1.8 ml. N₂H₄.H₂O with 0.4 g. Na in 9 ml. absolute EtOH in a sealed tube 14 hrs. at 170-80°, distilling the EtOH, refluxing the residue 4 hrs. with 10 ml. H₂O, acidifying with HCl, evaporating, heating the residue with 10 ml. 10% alc. HCl 3 hrs., distilling the EtOH, treating the residue with K₂CO₃, and extracting with Et₂O gave 0.17 g. 2-(2-carbethoxyethyl)quinuclidine, b_{0.2} 90-2°, which, refluxed 4 hrs. with 17% HCl, gave 0.06 g. 2-(2-carboxyethyl)quinuclidine HCl salt, decompose 216.5-17.5°. Reduction of II with LiAlH₄ in Et₂O gave 56.7% 3-hydroxy-2-(3-hydroxypropyl)quinuclidine, b_{0.4} 163-5°; HCl salt, m. 132-3°. Refluxing Ia with AcOH-concentrated HCl 17 hrs. gave 92% 3-oxo-2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 245° (90% EtOH). This refluxed 4 hrs. with 9% alc. HCl gave 63.6% 3-oxo-2,2-bis(2-carbethoxyethyl)quinuclidine (III), b₁ 190°, m. 58-61°; HCl salt, m. 169-71° (EtOH). Reductions of III with LiAlH₄ in Et₂O gave 85% 3-hydroxy-2,2-bis(3-hydroxypropyl)quinuclidine, hygroscopic crystals; HCl salt, m. 221-3° (EtOH). Keeping 0.35 g. III with 0.6 ml. N₂H₄.H₂O in 2 ml. absolute EtOH 8 days gave 0.2 g. III dihydrazide, hygroscopic solid yielding a picrate, decompose 168°. Heating III with N₂H₄.H₂O in EtOH-EtONa, as above, 14 hrs. at 160-70° gave 50% 2,2-bis(2-carbethoxyethyl)quinuclidine, b_{0.2} 175-80°, which, refluxed 4 hrs. with 17% HCl, gave 30% 2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 215-18° (Me₂CO-EtOH). Heating 1.2 g. LiAlH₄, 1 g. Ia, 45 ml. C₆H₆, and 20 ml. absolute Et₂O 40 hrs. at 65-70°, adding 3 ml. H₂O, separating the inorg.

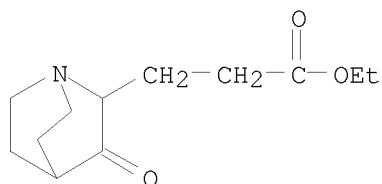
salts, washing these with dry pyridine, and evaporating the filtrate gave 59.6% 3-hydroxy-2,2-bis-(2-cyanoethyl)quinuclidine, m. 179-80° (absolute EtOH).

IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 75208-48-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI)
(CA INDEX NAME)



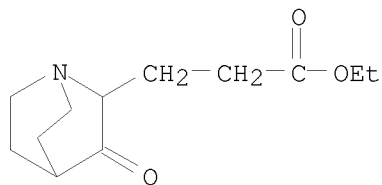
● HCl

RN 105339-98-8 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI)
(CA INDEX NAME)

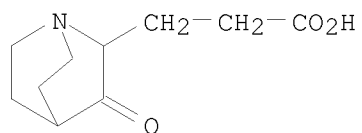


● HCl

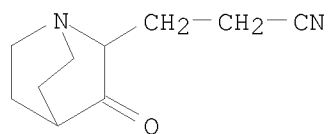
RN 105339-99-9 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



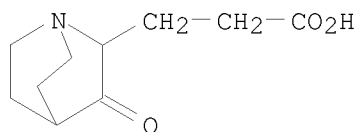
IT 117342-57-1, 2-Quinuclidinepropionic acid, 3-oxo-
(derivs.)
RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 99169-54-7P, 2-Quinuclidinepropionitrile, 3-oxo-
 RL: PREP (Preparation)
 (preparation of)
 RN 99169-54-7 CAPLUS
 CN 2-Quinuclidinepropionitrile, 3-oxo- (6CI) (CA INDEX NAME)

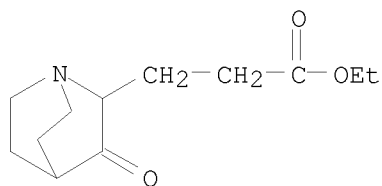


L15 ANSWER 133 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1959:122171 CAPLUS
 DOCUMENT NUMBER: 53:122171
 ORIGINAL REFERENCE NO.: 53:21953e-f
 TITLE: Syntheses in the allo-lupinane series. IV. An
 alternative synthesis of 4-hydroxymethylquinolizidine
 AUTHOR(S): Lukes, R.; Vesely, Z.
 CORPORATE SOURCE: Vysoka skola chem. technol., Prague
 SOURCE: Collection of Czechoslovak Chemical Communications (1959), 24, 2318-23
 CODEN: CCCCAK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB See C.A. 53, 368f.
 IT 75208-48-9 105339-98-8 105339-99-9
 (Derived from data in the 6th Collective Formula Index (1957-1961))
 RN 75208-48-9 CAPLUS
 CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI)
 (CA INDEX NAME)



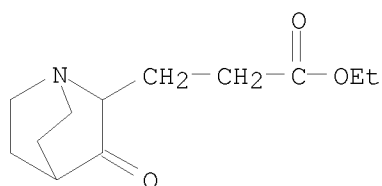
● HCl

RN 105339-98-8 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI)
 (CA INDEX NAME)



● HCl

RN 105339-99-9 CAPLUS
 CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



L15 ANSWER 134 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1940:708 CAPLUS
DOCUMENT NUMBER: 34:708
ORIGINAL REFERENCE NO.: 34:110b-g
TITLE: Synthesis of 5-substituted rubans
AUTHOR(S): Clemo, G. R.; Hoggarth, E.
SOURCE: Journal of the Chemical Society (1939)
1241-4
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 34:708

GI For diagram(s), see printed CA Issue.

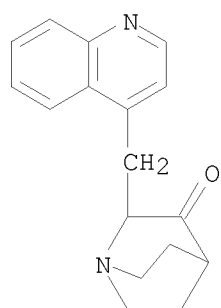
AB Lepidine (40 g.), 44 g. chloral and 100 cc. C₅H₅N, warmed at 85-90° for 2 hrs., give 80% of γ -trichloro- β -hydroxy- α -(4-quinolyl)propane, m. 178°; adding 65 g. during 2 hrs. to 65 g. KOH in 300 cc. absolute EtOH on the water bath gives 80% of β -4-quinolylacrylic acid, m. 270°; oxidation of 36 g. acid in a solution of 14 g. Na₂CO₃ in 500 cc. H₂O with 60 g. KMnO₄ in 1.5 l. H₂O at -10° gives 58% (overall yield 38-40%) of quinoline-4-aldehyde (I), b₄ 122-3°, m. 52°; picrate, yellow, m. 179° (contains 1 mole of EtOH). 3-Ketoquinuclidine (II) (C. and Metcalfe, C. A. 32, 1701.3, term it the 2-derivative) and BzH in absolute EtOH containing piperidine or

KOH, refluxed 8-10 hrs., give 2-benzylidene-3-ketoquinuclidine, light yellow, m. 133°; phenylhydrazone, light yellow, m. 184°. II (0.5 g.) and 0.8 g. I in AcOH, saturated with dry HCl at 0°, and after 2-3 hrs. warmed at 80-5° for 8 hrs., give 0.2 g. 5-keto-6,9-rubanene (III), deep yellow, m. 153°; III results in 0.4-0.5 g. yield from 0.5 g. II and 0.65 g. I with piperidine acetate in absolute EtOH; after keeping 60 hrs. in the cold and then heating momentarily to boiling; picrate, red, m. 209°; chloroplatinate, orange needles, decompose above 260° without melting. Catalytic reduction of 0.5 g. of III with Pd-C in MeOH gives 0.3 g. of 5-ketoruban (IV (R = 4-quinolyl)), m. 125-6°; phenylhydrazone, yellow, m. 198°; picrate, deep yellow, m. 168°. Reduction of 0.5 g. of IV with (iso-PrO)₃Al in iso-PrOH gives 0.3 g. of ruban-5-ol, m. 198°; picrate, yellow, m. 188-9°. IV (0.3 g.) with EtMgI in Et₂O at -10° gives 0.03-0.05 g. of 5-ethylruban-5-ol (V), m. 139°; picrate, yellow, m. 161°. III (0.8 g.) and EtMgI in Et₂O at 0° give 0.05 g. of a compound C₁₉H₂₂ON₂, m. 164°; picrate, deep yellow, m. 150°; crystalline compds. could not be prepared with N₂H₄.H₂O, PhNHNH₂, NH₂OH or H₂NNHCONH₂; no Me₂CO was detected in an attempted reduction with (iso-PrO)₃Al and the compound was unchanged on boiling with HCO₂H or Ac₂O; catalytic reduction did not yield V.

IT 24177-70-6, 3-Quinuclidinone, 2-(4-quinolylmethyl)-
(and derivs.)

RN 24177-70-6 CAPLUS

CN 11-Norcinchonan-7-one, (8 ξ)-(9CI) (CA INDEX NAME)



=> FIL STNGUIDE
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
324.97	861.18

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
-44.80	-44.80

CA SUBSCRIBER PRICE

FILE 'STNGUIDE' ENTERED AT 15:17:16 ON 11 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 6, 2008 (20080606/UP).

=> log y
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
1.26	862.44

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
0.00	-44.80

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 15:29:48 ON 11 JUN 2008